Supporting Information

Practical heterogeneous photoredox/nickel dual catalysis for C-N and C-O coupling reactions

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1. General information

Unless otherwise noted, materials were purchased from commercial suppliers and used without further purification. All the solvents were treated according to standard methods.[1] Flash column chromatography was performed using 200-300 mesh silica gel. ^{1}H NMR spectra were recorded on 400 or 600 MHz spectrophotometers. Chemical shifts (δ (ppm)) are reported in ppm from the resonance of tetramethyl silane as the internal standard (TMS: 0.00 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, dd = doublet of doublets, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR spectra were recorded on 100 MHz with complete proton decoupling spectrophotometers ($CDCl_3$: 77.0 ppm,).

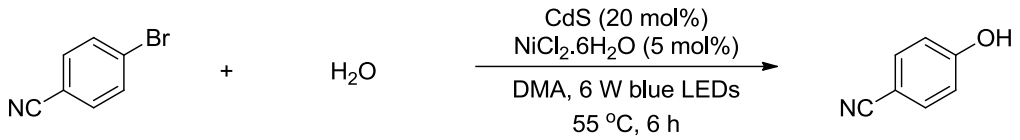
2. Detailed Condition Optimization

Table S1 Condition optimization for the C-O coupling of aryl bromides with alcohols[a]

entry	variation from the standard conditions	yield (%)[b]
1[c]	none	96
2	no CdS	0
3	no $NiCl_2.6H_2O$	0
4	no dtbbpy	trace
5	no Et_3N	trace
6[c]	in air	0
7	in the dark	0
8	MeCN instead of DMA	65
9	$NiCl_2$.glyme instead of $NiCl_2.6H_2O$	96
10	K_2CO_3 instead of Et_3N	0
11	5.0 equiv. of MeOH	71

[a]Conditions: **1b** (1.0 mmol), CdS (0.05 mmol, 5 mol%), $NiCl_2$•$6H_2O$ (0.06 mmol, 6 mol%), dtbbpy (0.02 mmol, 2 mol%), MeOH (2.0 mL) and DMA (1.0 mL) under irradiation with 6 W blue LEDs. [b]Isolated yield of **5ba**.

Table S2. Condition optimization for hydroxylation of aryl bromide[a]



1b, 1.0 mmol 10.0 eq. **6b**

entry	variation of the standard conditions	yield (%)[b]
1	none	85
2	no CdS	0
3	no $NiCl_2 \cdot 6H_2O$	0
4	in air	0
5	in the dark	0
6	MeCN instead of DMA	73
7	$NiCl_2$·glyme instead of $NiCl_2 \cdot 6H_2O$	86
8	5 mol% dtbbpy as ligand	86
9	at room temperature	0

[a]Reaction conditions: **1b** (1.0 mmol), water (10.0 mmol, 10.0 equiv), CdS (0.20 mmol, 20 mol%), $NiCl_2 \cdot 6H_2O$ (0.05 mmol, 5 mol%) and DMA (2.0 mL) under irradiation by 6 W blue LEDs. [b]Isolated yield.

3. General Procedure and Spectral Data of Products

3.1 General procedure 1: C-N coupling reaction

Aryl bromide (1.0 equiv.), amine (2.0 equiv.), CdS (20 mol%), $NiCl_2 \cdot 6H_2O$ (5 mo%) and DMA (3 mL) were added to a 10 mL Schlenk flask equipped with a magnetic stir bar. The mixture was treated with ultrasonic for 10s. Then it was subjected to the "freeze-pump-thaw" procedure for 2 times. After that, the reaction mixture was sitrred under the irradiation of a 6 W blue LEDs (distance ca. 5 cm), either under fan cooling (to maintain ambient temperature) or without fan cooling (to heat to approximately 55 °C). Upon the completion of reaction as monitored by TLC, the reaction mixture was diluted with water (10 mL) and extracted with Et_2O (3 × 15 mL). The organic extracts were washed with brine (10 mL) and the combined aqueous layers were extracted once more with Et_2O (10 mL). The combined organic extracts were dried over $MgSO_4$ and concentrated in vacuo. Purification of the crude product by flash chromatography on silica gel using the indicated solvent system afforded the desired product.

3.2 General procedure 2: C-O coupling reaction

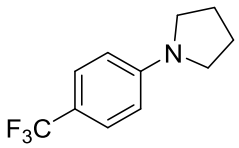
Aryl bromide (1.0 equiv.), CdS (5 mol%), $NiCl_2 \cdot 6H_2O$ (6 mo%), dtbbpy (5 mol%), Et_3N (2.0 equiv.), MeOH (2.0 mL) and DMA (1.0 mL) were added to a 10 mL Schlenk flask equipped with a magnetic stir bar. The mixture was treated with ultrasonic for 10s. Then it was subjected to the "freeze-pump-thaw" procedure for 2 times. After that, the reaction mixture was sitrred at room temperature under the irradiation of a 6 W blue LEDs (distance ca. 5 cm). Upon the completion of reaction as monitored by TLC, the reaction mixture was diluted with water (10 mL) and extracted with Et_2O (3 × 15 mL). The organic extracts were washed with brine (10 mL) and the combined aqueous layers were extracted once more with Et_2O (10 mL). The combined organic extracts were dried over $MgSO_4$ and concentrated in vacuo. Purification of the crude product by flash chromatography on silica gel using the indicated solvent system afforded the desired product.

3.3 General procedure 3: hydroxylation reaction

Aryl bromide (1.0 equiv.), H_2O (10.0 equiv.), CdS (20 mol%), $NiCl_2 \cdot 6H_2O$ (5 mo%) and DMA (3 mL)were added to a 10 mL Schlenk flask equipped with a magnetic stir bar. The mixture was treated with ultrasonic for 10s. Then it was subjected to the "freeze-pump-thaw" procedure for 2 times. After that, the reaction mixture was sitrred under the irradiation of a 6 W blue LEDs (distance ca. 5 cm). The reaction vial was heated to roughly 55 °C by the blue LEDs without the use of a fan. Upon the completion of reaction as monitored by TLC, the reaction mixture was diluted with water (10 mL) and extracted with Et_2O (3 × 15 mL). The organic extracts were washed with brine (10 mL) and the combined aqueous layers were extracted once more with Et_2O (10 mL). The combined organic extracts were dried over $MgSO_4$ and concentrated in vacuo. Purification of the crude product by flash chromatography on silica gel using the indicated solvent system afforded the desired product.

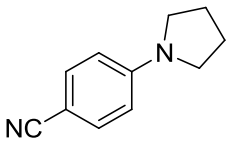
3.4 Spectral data of products

1-(4-(Trifluoromethyl)phenyl)pyrrolidine (3aa)[2]



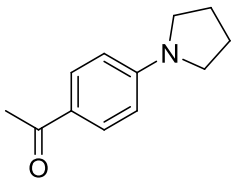
Prepared according to general procedure 1 (rt): white solid, 178.2 mg, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) δ = 7.43 (d, *J* = 8.1 Hz, 2H), 6.54 (d, *J* = 8.1 Hz, 2H), 3.32 (t, *J* = 5.2 Hz, 4H), 2.03 (t, *J* = 5.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 149.7, 126.3 (q, *J* = 3.7 Hz), 125.3 (q, *J* = 268.2 Hz), 116.5 (q, *J* = 32.5 Hz), 110.8, 47.5, 25.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -60.5 (s, 3F).

4-(Pyrrolidin-1-yl)benzonitrile (3ba)[3]



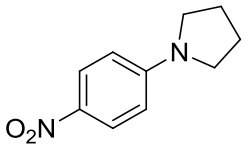
Prepared according to general procedure 1 (rt): white solid, 155 mg, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.44 (d, *J* = 8.3 Hz, 2H), 6.50 (d, *J* = 8.2 Hz, 2H), 3.32 (t, *J* = 4.9 Hz, 4H), 2.05 (t, *J* = 4.9 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 149.8, 133.2, 120.9, 111.3, 96.2, 47.3, 25.3.

1-(4-(Pyrrolidin-1-yl)phenyl)ethanone (3ca)[4]



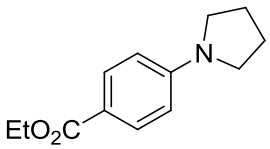
Prepared according to general procedure 1 (rt): white solid, 151 mg, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.86 (d, *J* = 8.3 Hz, 2H), 6.51 (d, *J* = 8.3 Hz, 2H), 3.36 (t, *J* = 5.7 Hz, 4H), 2.50 (s, 3H), 2.03 (t, *J* = 5.7 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 196.3, 150.9, 130.6, 124.8, 110.6, 47.5, 25.9, 25.4.

1-(4-Nitrophenyl)pyrrolidine (3da)[5]



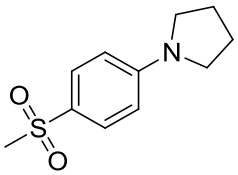
Prepared according to general procedure 1 (rt): yellow solid, 119 mg, 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.10 (d, *J* = 9.3 Hz, 2H), 6.45 (d, *J* = 9.3 Hz, 2H), 3.40 (t, *J* = 6.5 Hz, 4H), 2.08 (t, *J* = 6.6 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.8, 136.3, 126.3, 110.3, 47.8, 25.4.

Ethyl 4-(pyrrolidin-1-yl)benzoate (3ea)[6]



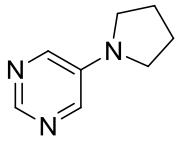
Prepared according to general procedure 1 (rt): white solid, 184 mg, 84% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.90 (d, *J* = 8.1 Hz, 2H), 6.50 (d, *J* = 8.2 Hz, 2H), 4.31 (q, *J* = 7.0 Hz, 2H), 3.35 (d, *J* = 5.1 Hz, 4H), 2.03 (t, *J* = 5.1 Hz, 4H), 1.36 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.1, 150.7, 131.2, 116.5, 110.5, 60.0, 47.4, 25.4, 14.4.

1-(4-(Methylsulfonyl)phenyl)pyrrolidine (3fa)[7]



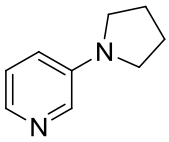
Prepared according to general procedure 1 (rt): white solid, 216 mg, 96% yield. mp: 161-163 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.73 (d, *J* = 8.1 Hz, 2H), 6.57 (d, *J* = 8.3 Hz, 2H), 3.36 (t, *J* = 4.7 Hz, 4H), 3.00 (s, 3H), 2.06 (t, *J* = 5.1 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 150.8, 129.0, 124.8, 110.9, 47.5, 45.1, 25.3. HRMS (ESI) for: $C_{11}H_{115}NO_2S$ $[M + H]^+$: calcd: 226.0896, found: 226.0895.

5-(Pyrrolidin-1-yl)pyrimidine (3ga)[8]



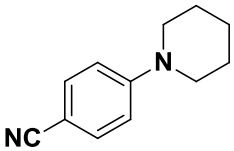
Prepared according to general procedure 1 (rt): colorless oil, 146 mg, 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.55 (s, 1H), 8.05 (s, 2H), 3.32 (t, *J* = 4.7 Hz, 4H), 2.06 (t, *J* = 4.7 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 146.6, 141.1, 139.3, 46.8, 25.2.

3-(Pyrrolidin-1-yl)pyridine (3ha)[4]



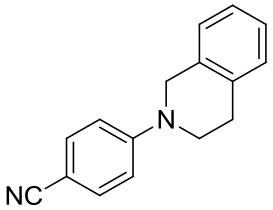
Prepared according to general procedure 1 (rt): colorless oil, 141 mg, 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.98 (s, 1H), 7.92 (d, *J* = 4.5 Hz, 1H), 7.10 (dd, *J* = 8.3, 4.6 Hz, 1H), 6.80 (d, *J* = 8.3 Hz, 1H), 3.29 (t, *J* = 6.0 Hz, 4H), 2.02 (t, *J* = 6.2 Hz, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 143.6, 136.8, 134.3, 123.4, 117.6, 47.2, 25.3.

4-(Piperidin-1-yl)benzonitrile (3bb)[9]



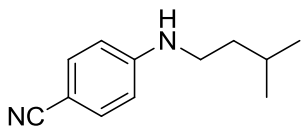
Prepared according to general procedure 1 (rt): white solid, 174 mg, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.46 (d, *J* = 8.0 Hz, 2H), 6.84 (d, *J* = 8.0 Hz, 2H), 3.33 (s, 4H), 1.66 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.4, 133.3, 120.3, 113.9, 98.5, 48.2, 25.1, 24.1.

4-(3,4-Dihydroisoquinolin-2(1H)-yl)benzonitrile (3bc)[10]



Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): white solid, 215 mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.52 (d, *J* = 8.5 Hz, 2H), 7.24 – 7.18 (m, 4H), 6.86 (d, *J* = 8.6 Hz, 2H), 4.50 (s, 2H), 3.63 (t, *J* = 5.8 Hz, 2H), 2.99 (t, *J* = 5.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 152.1, 134.9, 133.5, 133.4, 128.1, 126.9, 126.5, 126.4, 120.4, 112.6, 98.6, 48.7, 44.5, 28.9.

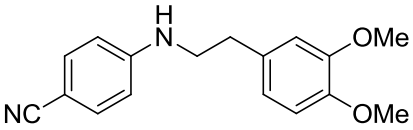
4-(Isopentylamino)benzonitrile (3bd)



Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): white solid, 177 mg, 94% yield. mp: 51-52 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ

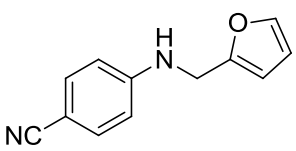
(ppm) 7.39 (d, *J* = 8.7 Hz, 2H), 6.54 (d, *J* = 8.7 Hz, 2H), 4.33 (s, 1H), 3.16 – 3.11 (m, 2H), 1.71 (dt, *J* = 13.3, 6.7 Hz, 1H), 1.52 (dd, *J* = 14.6, 7.1 Hz, 2H), 0.95 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.5, 133.5, 120.6, 111.9, 97.7, 41.2, 37.8, 25.7, 22.4. IR (in KBr): 2962, 2922, 2862, 2206, 1606, 1529, 1473, 1338, 1171, 823 cm^{-1}. HRMS (ESI) for: $C_{12}H_{17}N_2$ $[M + H]^+$: calcd: 189.1386, found: 189.1384.

4-((3,4-Dimethoxyphenethyl)amino)benzonitrile (3be)



Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): white solid, 251 mg, 89% yield. mp: 119-120 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.41 (d, *J* = 8.7 Hz, 2H), 6.79 (dd, *J* = 32.8, 8.1 Hz, 2H), 6.71 (s, 1H), 6.55 (d, *J* = 8.8 Hz, 2H), 4.25 (d, *J* = 4.3 Hz, 1H), 3.86 (d, *J* = 4.4 Hz, 6H), 3.42 (q, *J* = 6.7 Hz, 2H), 2.87 (t, *J* = 6.9 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.0, 149.1, 147.8, 133.7, 130.8, 120.6, 120.4, 112.2, 111.8, 111.4, 98.7, 55.9, 55.8, 44.2, 34.6. IR (in KBr): 2938, 2837, 2362, 2208, 1605, 1519, 1460, 1337, 1220, 1119, 616 cm^{-1}. HRMS (ESI) for: $C_{17}H_{19}N_2O_2$ $[M + H]^+$: calcd: 283.1441, found: 283.1435.

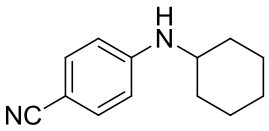
4-((Furan-2-ylmethyl)amino)benzonitrile (3bf)[11]



Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): white solid, 186 mg, 94% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.42 (d, J = 8.7 Hz, 2H), 7.37 (d, J = 0.7 Hz, 1H), 6.63 (d, J = 8.7 Hz, 2H), 6.34 – 6.33 (m, 1H), 6.25 (d, J = 3.1 Hz, 1H), 4.65 (s, 1H), 4.35 (d, J = 5.7 Hz, 2H).

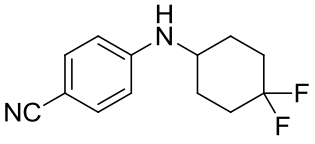
^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.1, 150.6, 142.3, 133.6, 120.3, 112.4, 110.4, 107.5, 99.3, 40.4.

4-(Cyclohexylamino)benzonitrile (3bg)[12]



Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): white solid, 145 mg, 73% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.38 (d, *J* = 8.7 Hz, 2H), 6.52 (d, *J* = 8.7 Hz, 2H), 4.19 (s, 1H), 3.28 (s, 1H), 2.02 (d, *J* = 12.6 Hz, 2H), 1.77 (dd, *J* = 9.8, 3.6 Hz, 2H), 1.66 (dd, *J* = 9.1, 3.6 Hz, 1H), 1.42 – 1.33 (m, 2H), 1.27 – 1.14 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 150.4, 133.6, 120.6, 112.2, 97.6, 51.1, 32.8, 25.6, 24.7.

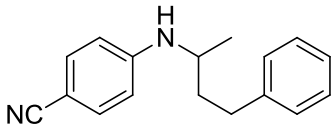
4-((4,4-Difluorocyclohexyl)amino)benzonitrile (3bh)



Prepared according to general procedure 1 (55 °C, and 4.0 equiv. of DBU): white solid, 200 mg, 85% yield. mp: 95-96 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.42 (d, *J* = 8.7 Hz, 2H), 6.56 (d, *J* = 8.7 Hz, 2H), 4.24 (s, 1H), 3.47 (s, 1H), 2.16 – 2.08 (m, 4H), 1.98 – 1.82 (m, 2H), 1.65 – 1.56 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm)

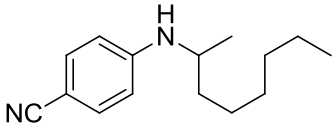
150.0, 133.7, 123.6 (t, *J* = 241.2 Hz), 120.3, 112.4, 98.7, 49.0, 31.84 (t, *J* = 24.9 Hz), 28.3 (d, *J* = 8.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -97.8 (dd, *J* = 1738.9, 239.3 Hz). IR (in KBr): 2953, 2206, 1601, 1522, 1347, 1175, 1123, 953, 821 cm^{-1}. HRMS (ESI) for: $C_{13}H_{15}F_2N_2$ $[M + H]^+$: calcd: 237.1198, found: 237.1195.

4-((4-Phenylbutan-2-yl)amino)benzonitrile (3bi)



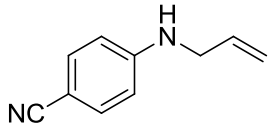
Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): colorless oil, 238 mg, 95% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.38 (d, *J* = 8.8 Hz, 2H), 7.29 (t, *J* = 7.3 Hz, 2H), 7.22 – 7.15 (m, 3H), 6.44 (d, *J* = 8.8 Hz, 2H), 4.00 (d, *J* = 7.8 Hz, 1H), 3.54 – 3.47 (m, 1H), 2.72 (dd, *J* = 14.5, 8.0 Hz, 2H), 1.91 – 1.79 (m, 2H), 1.24 (d, *J* = 6.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 150.5, 141.3, 133.7, 128.5, 128.4, 126.1, 120.5, 112.3, 98.2, 47.4, 38.3, 32.3, 20.5. IR (in KBr): 2971, 2931, 2211, 1605, 1447, 1342, 1173, 826, 748, 702, 545 cm^{-1}. HRMS (ESI) for: $C_{17}H_{19}N_2$ $[M + H]^+$: calcd: 251.1543, found: 251.1539.

4-(Octan-2-ylamino)benzonitrile (3bj)



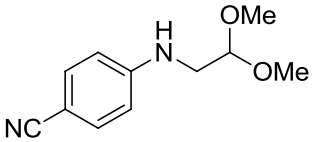
Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): colorless oil, 193 mg, 83% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.39 (dd, *J* = 8.3, 6.9 Hz, 2H), 6.52 (dd, *J* = 8.4, 5.7 Hz, 2H), 4.09 (dd, *J* = 77.9, 7.5 Hz, 1H), 3.49 (dt, *J* = 13.2, 6.5 Hz, 1H), 1.56 – 1.28 (m, 10H), 1.19 (d, *J* = 6.3 Hz, 3H), 0.88 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 150.7, 133.8, 120.6, 112.2, 97.9, 48.2, 36.9, 31.8, 29.2, 26.0, 22.6, 20.5, 14.0. IR (in KBr): 2931, 2857, 2216, 1609, 1526, 1458, 1338, 1168, 830, 541 cm^{-1}. HRMS (ESI) for: $C_{15}H_{23}N_2$ $[M + H]^+$: calcd: 231.1856, found: 231.1854.

4-(Allylamino)benzonitrile (3bk)[4]



Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): colorless oil, 128 mg, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.42 (d, *J* = 8.4 Hz, 2H), 6.57 (d, *J* = 8.2 Hz, 2H), 6.03 – 5.77 (m, 1H), 5.25 (dd, *J* = 24.9 Hz, 13.7, 2H), 4.39 (s, 1H), 3.82 (t, *J* = 5.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.0, 133.7, 133.6, 120.4, 117.0, 112.3, 98.8, 45.6.

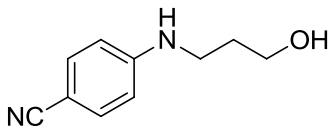
4-((2,2-Dimethoxyethyl)amino)benzonitrile (3bl)



Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): colorless oil, 198 mg, 96% yield. mp: 61-62 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.42 (d, *J* = 8.8 Hz, 2H), 6.59 (d, *J* = 8.8 Hz, 2H), 4.55 (t, *J* = 5.3 Hz,

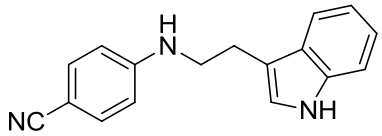
1H), 4.44 (s, 1H), 3.42 (s, 6H), 3.29 (d, *J* = 5.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.0, 133.6, 120.3, 112.3, 102.0, 98.9, 54.0, 44.5. IR (in KBr): 2916, 2207, 1609, 1522, 1478, 1340, 1127, 1070, 973, 822, 618 cm^{-1}. HRMS (ESI) for: $C_{11}H_{15}N_2O_2$ $[M + H]^+$: calcd: 207.1128, found: 207.1127.

4-((3-Hydroxypropyl)amino)benzonitrile (3bm)



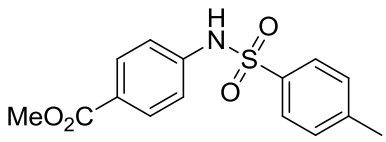
Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): white solid, 160 mg, 91% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.41 (d, *J* = 8.7 Hz, 2H), 6.56 (d, *J* = 8.7 Hz, 2H), 3.83 (t, *J* = 5.7 Hz, 2H), 3.32 (t, *J* = 6.5 Hz, 2H), 1.90 (p, *J* = 6.2 Hz, 2H), 1.63 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.5, 133.6, 120.6, 112.1, 98.0, 61.0, 40.9, 31.2. IR (in KBr): 3299, 2935, 2838, 2218, 1610, 1531, 1344, 1117, 830, 618 cm^{-1}. HRMS (ESI) for: $C_{10}H_{13}N_2O$ $[M + H]^+$: calcd: 177.1022, found: 177.1022.

4-((2-(1H-indol-3-yl)ethyl)amino)benzonitrile (3bn)



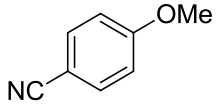
Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): white solid, 256 mg, 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.11 (s, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 7.38 (d, *J* = 8.8 Hz, 3H), 7.24 – 7.12 (m, 2H), 7.03 (d, *J* = 1.9 Hz, 1H), 6.51 (d, *J* = 8.8 Hz, 2H), 4.29 (s, 1H), 3.48 (t, *J* = 6.7 Hz, 2H), 3.08 (t, *J* = 6.7 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 151.2, 136.4, 133.6, 127.2, 122.3, 122.1, 120.6, 119.6, 118.5, 112.5, 112.2, 111.4, 98.4, 43.1, 24.8. IR (in KBr): 2204, 1602, 1528, 1341, 1174, 1110, 827, 752, 620 cm^{-1}. HRMS (ESI) for: C17H16N3 $[M + H]^+$: calcd: 262.1339, found: 262.1337.

Methyl 4-(4-methylphenylsulfonamido)benzoate (3io)[13]



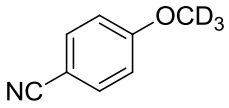
Prepared according to general procedure 1 (55 °C, and 2.0 equiv. of DBU): white solid, 245 mg, 90% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.91 (d, *J* = 8.7 Hz, 2H), 7.71 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.7 Hz, 2H), 6.95 (s, 1H), 3.87 (s, 3H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 166.4, 143.5, 142.2, 136.5, 130.7, 129.5, 127.0, 125.0, 118.4, 51.8, 21.3.

4-Methoxybenzonitrile (5ba)[14]



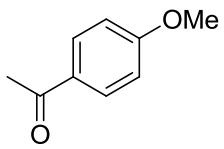
Prepared according to general procedure 2: white solid, 132 mg, 99% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.59 (d, *J* = 8.8 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.8, 134.0, 119.2, 114.7, 103.9, 55.5.

Deuterated 4-methoxybenzonitrile (5bb)[14]



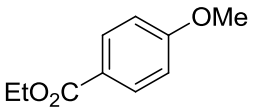
Prepared according to general procedure 2: white solid, 95 mg, 70% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.58 (d, *J* = 8.9 Hz, 2H), 6.95 (d, *J* = 8.9 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.8, 133.9, 119.2, 114.7, 103.8, 54.7 (dt, *J* = 44.0, 22.1 Hz).

1-(4-Methoxyphenyl)ethanone (5ca)[14]



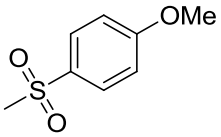
Prepared according to general procedure 2: white solid, 138 mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.94 (d, *J* = 8.9 Hz, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H), 2.56 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 196.8, 163.4, 130.5, 130.3, 113.6, 55.4, 26.3.

Ethyl 4-methoxybenzoate (5ea) [14]



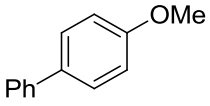
Prepared according to general procedure 2: white solid, 128 mg, 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 8.00 (d, *J* = 8.4 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 4.35 (q, *J* = 7.1 Hz, 2H), 3.86 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 166.4, 163.2, 131.5, 122.9, 113.5, 60.69, 55.4, 14.3.

1-Methoxy-4-(methylsulfonyl)benzene (5fa)[15]



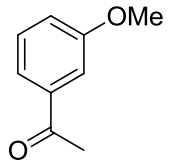
Prepared according to general procedure 2: white solid, 174 mg, 93% yield, ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.87 (d, *J* = 8.5 Hz, 2H), 7.03 (d, *J* = 8.5 Hz, 2H), 3.89 (s, 3H), 3.04 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 163.6, 132.2, 129.5, 114.4, 55.7, 44.8.

4-Methoxy-1,1'-biphenyl (5ja)[16]



Prepared according to general procedure 2: white solid, 128 mg, 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.56-7.51 (m, 4H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 8.7 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 159.1, 140.8, 133.7, 128.7, 128.1, 126.7, 126.6, 114.2, 55.3.

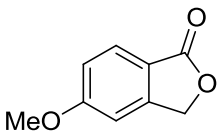
1-(3-Methoxyphenyl)ethanone (5ka)[17]



Prepared according to general procedure 2: colorless oil, 160 mg, 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.54 (d, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 2.2 Hz, 1H), 7.37 (t, *J* = 7.9 Hz, 1H), 7.12 – 7.10 (m, 1H), 3.85 (s, 3H), 2.60 (s, 3H). ^{13}C NMR (100 MHz,

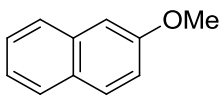
$CDCl_3$) δ (ppm) 197.9, 159.7, 138.4, 129.5, 121.1, 119.6, 112.2, 55.4, 26.7.

5-Methoxyisobenzofuran-1(3H)-one (5la)[18]



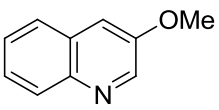
Prepared according to general procedure 2: white solid, 160 mg, 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.84 – 7.80 (m, 1H), 7.04 (d, *J* = 8.2 Hz, 1H), 6.93 (s, 1H), 5.26 (s, 2H), 3.91 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 170.8, 164.6, 149.3, 127.2, 118.0, 116.5, 105.9, 69.1, 55.8.

2-Methoxynaphthalene (5ma)[19]



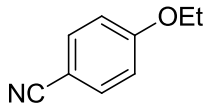
Prepared according to general procedure 2: white solid, 157 mg, 99% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.81 – 7.68 (m, 3H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.15 (d, *J* = 7.8 Hz, 2H), 3.93 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 157.5, 134.5, 129.4, 128.9, 127.6, 126.7, 126.4, 123.6, 118.7, 105.6, 55.3.

3-Methoxyquinoline (5na)[20]



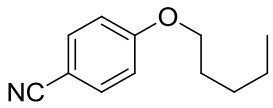
Prepared according to general procedure 2: colorless oil, 154 mg, 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 8.68 (d, *J* = 2.9 Hz, 1H), 8.05 (d, *J* = 8.2 Hz, 1H), 7.72 (d, *J* = 8.0 Hz, 1H), 7.57 – 7.48 (m, 2H), 7.37 (d, *J* = 2.6 Hz, 1H), 3.94 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 153.0, 144.6, 143.5, 129.1, 128.8, 127.0, 126.6, 126.6, 112.1, 55.4.

4-Ethoxybenzonitrile (5bc)[14]



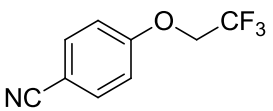
Prepared according to general procedure 2: white solid, 142 mg, 97% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.58 (d, *J* = 8.7 Hz, 2H), 6.93 (d, *J* = 8.7 Hz, 2H), 4.08 (q, *J* = 7.0 Hz, 2H), 1.44 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.2, 133.9, 119.3, 115.1, 103.6, 63.9, 14.5.

4-(Pentyloxy)benzonitrile (5bd)[21]



Prepared according to general procedure 2: colorless oil, 166 mg, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.57 (d, *J* = 8.9 Hz, 2H), 6.93 (d, *J* = 8.9 Hz, 2H), 3.99 (t, *J* = 6.5 Hz, 2H), 1.84 – 1.77 (m, 2H), 1.48 – 1.34 (m, 4H), 0.94 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 162.4, 133.9, 119.3, 115.1, 103.6, 68.4, 28.6, 28.0, 22.3, 13.9.

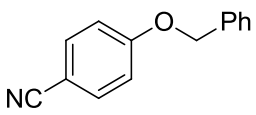
Ethyl 4-methoxybenzoate (5be)[22]



Prepared according to general procedure 2: white solid, 193 mg, 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.65 (d, *J* = 9.0 Hz, 2H), 7.02 (d, *J* = 8.9 Hz, 2H), 4.42

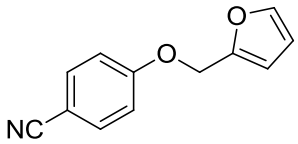
(q, *J* = 7.9 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.2, 134.2, 122.8 (q, *J* = 278.0 Hz), 118.5, 115.4, 106.1, 65.5 (q, *J* = 36.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -73.8 (s, 3F).

4-(Benzyloxy)benzonitrile (5bf)[23]



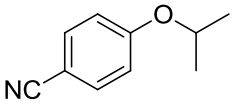
Prepared according to general procedure 2: white solid,194 mg, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.58 (d, *J* = 8.5 Hz, 2H), 7.46 – 7.32 (m, 5H), 7.02 (d, *J* = 8.4 Hz, 2H), 5.11 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 161.9, 135.6, 134.0, 128.7, 128.4, 127.4, 119.1, 115.5, 104.1, 70.2.

4-(Furan-2-ylmethoxy)benzonitrile (5bg)[24]



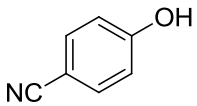
Prepared according to general procedure 2: white solid, 191 mg, 96% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.59 (d, *J* = 8.9 Hz, 2H), 7.47 (d, *J* = 1.0 Hz, 1H), 7.04 (d, *J* = 8.9 Hz, 2H), 6.48 (d, *J* = 3.2 Hz, 1H), 6.40 (dd, *J* = 3.1, 1.8 Hz, 1H), 5.05 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 161.4, 148.9, 143.5, 133.9, 119.1, 115.4, 110.7, 110.6, 104.4, 62.34.

4-Isopropoxybenzonitrile (5bh)[25]



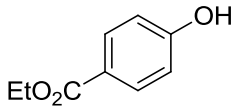
Prepared according to general procedure 2: colorless oil, 87 mg, 54% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.56 (d, *J* = 8.9 Hz, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 4.62 (hept, *J* = 6.1 Hz, 1H), 1.36 (d, *J* = 6.1 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 161.9, 135.6, 134.0, 128.7, 128.4, 127.4, 119.1, 115.5, 104.1, 70.2.

4-Hydroxybenzonitrile (6b)[26]



Prepared according to general procedure 3: white solid, 101 mg, 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.56 (d, *J* = 8.8 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 160.4, 134.3, 119.2, 116.5, 102.7.

Ethyl 4-hydroxybenzoate (6e)[26]



Prepared according to general procedure 3: white solid, 145 mg, 87% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm). 7.96 (d, *J* = 8.5 Hz, 2H), 6.88 (d, *J* = 8.5 Hz, 2H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.5, 160.7, 131.9, 122.0, 115.3, 61.2, 14.2.

4. Reusability of CdS.

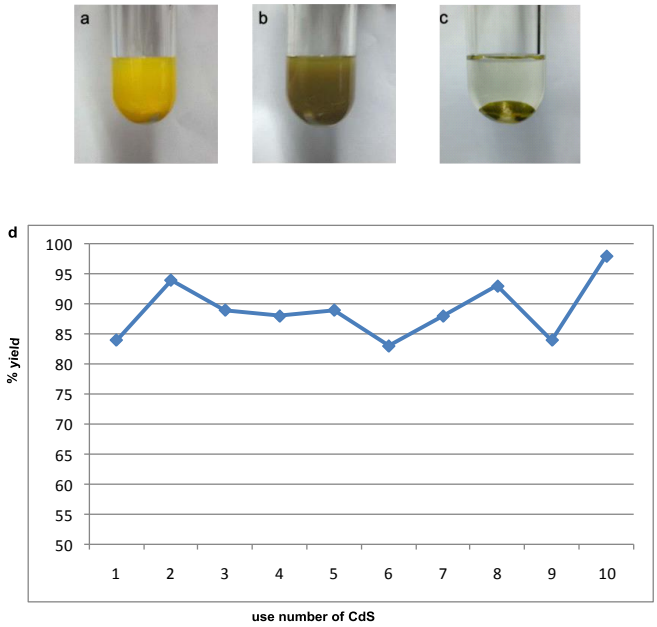


Figure S1. Reusability of CdS. (a) Before and (b) after the C-N coupling reaction, (c) the catalyst settles down and is attracted, and (d) the yield of product **3aa** with the use of recycled photocatalyst CdS.

5. Unsuitable examples

Figure S2. Selected examples of unsuitable aryl bromides in the C-N coupling conditions.

6. References

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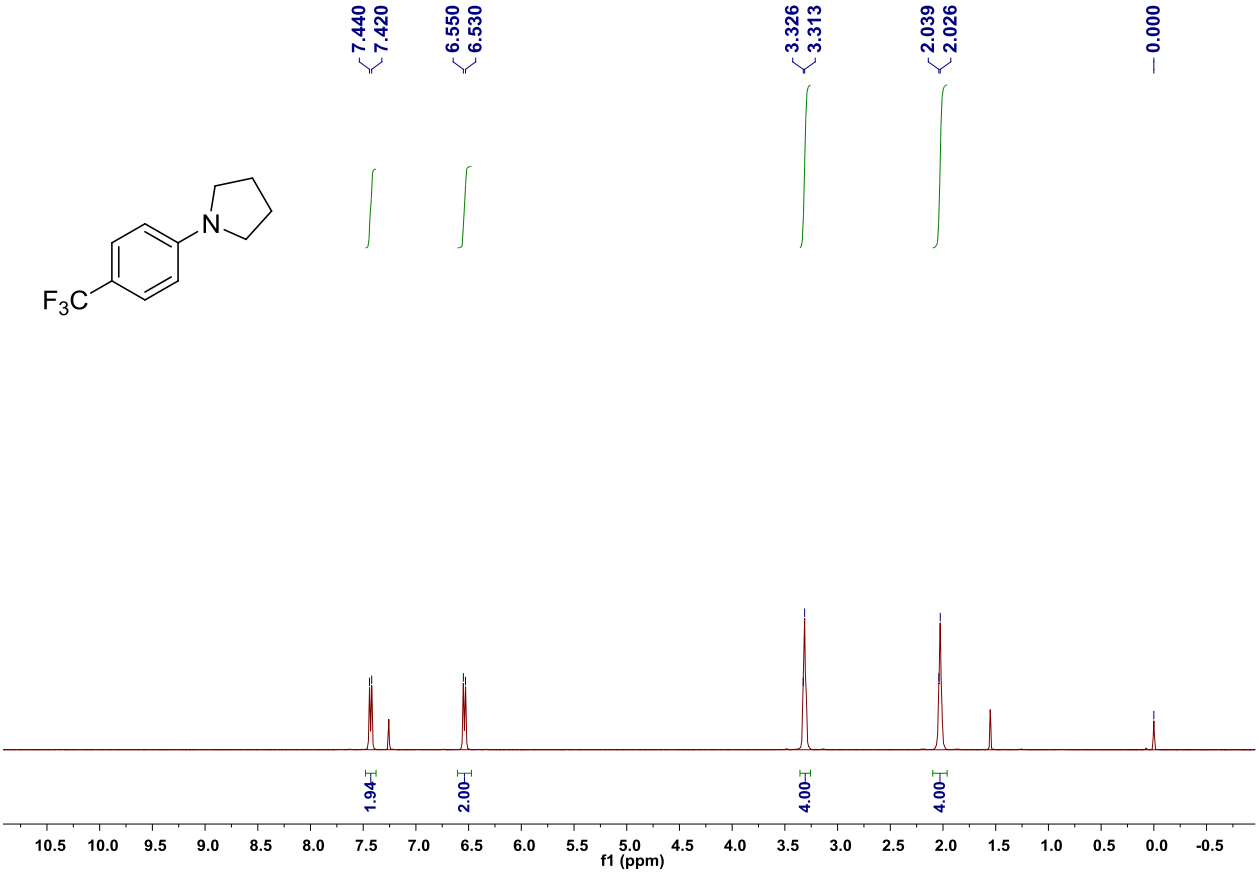
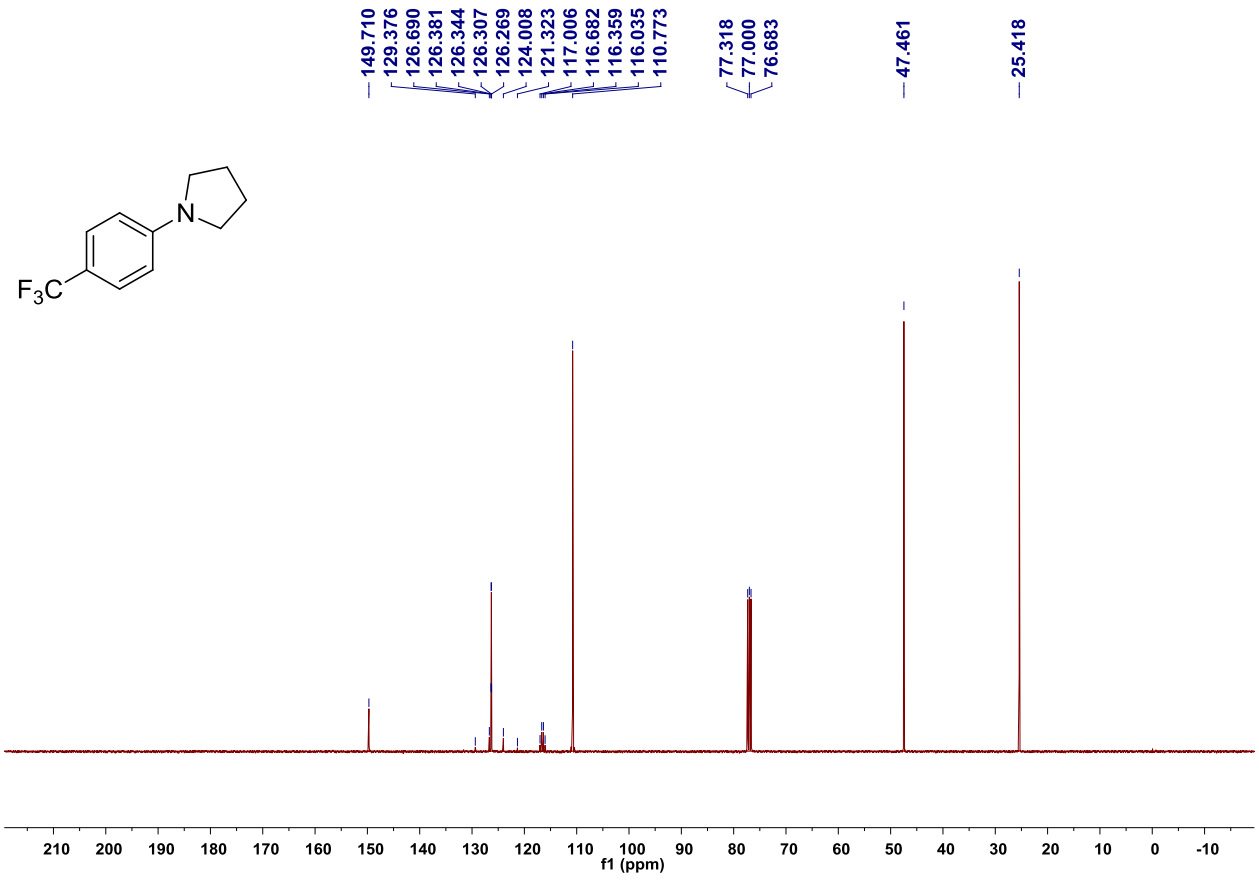
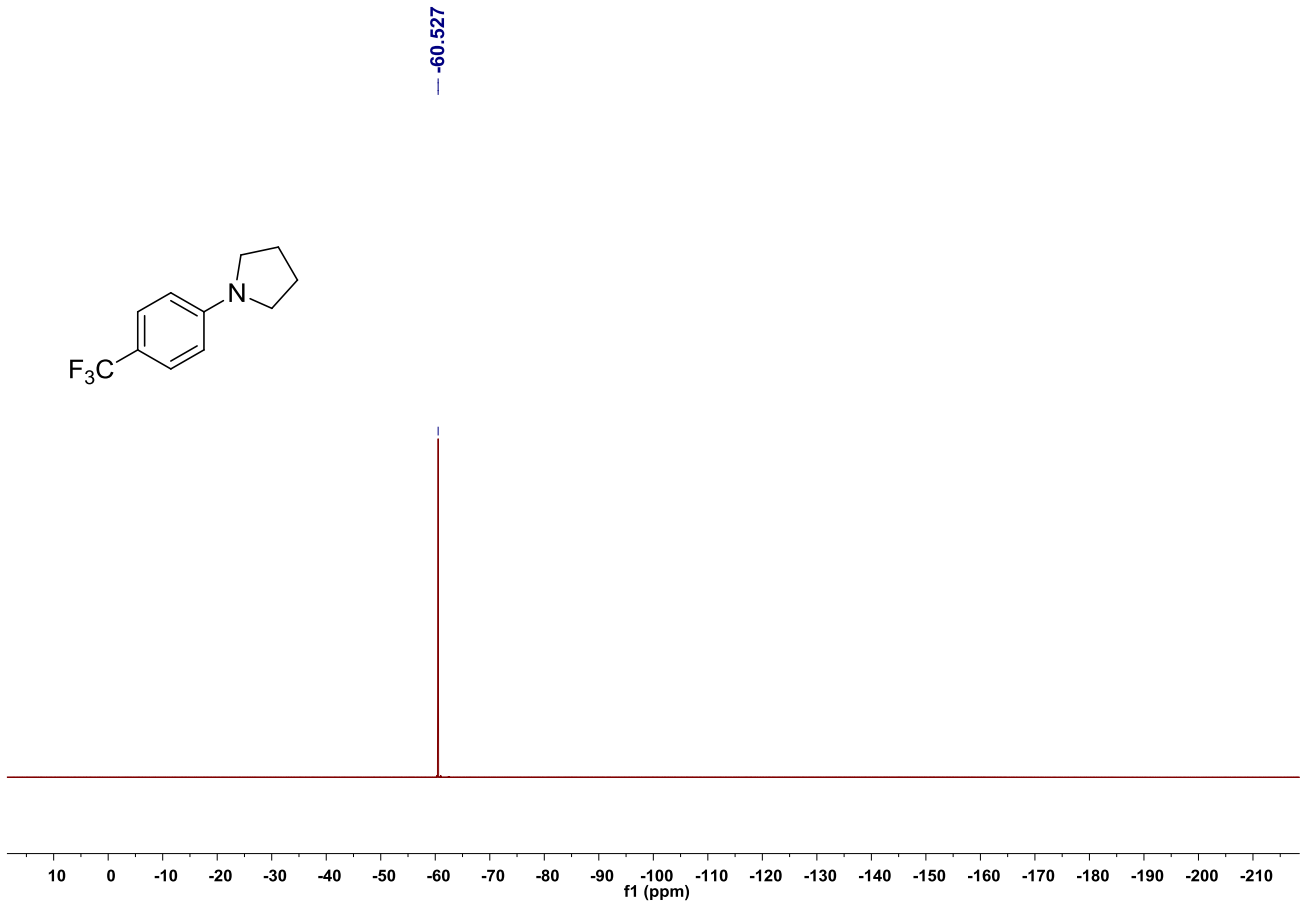
7. Copies of ^{1}H NMR and ^{13}C NMR Spectra



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F3C
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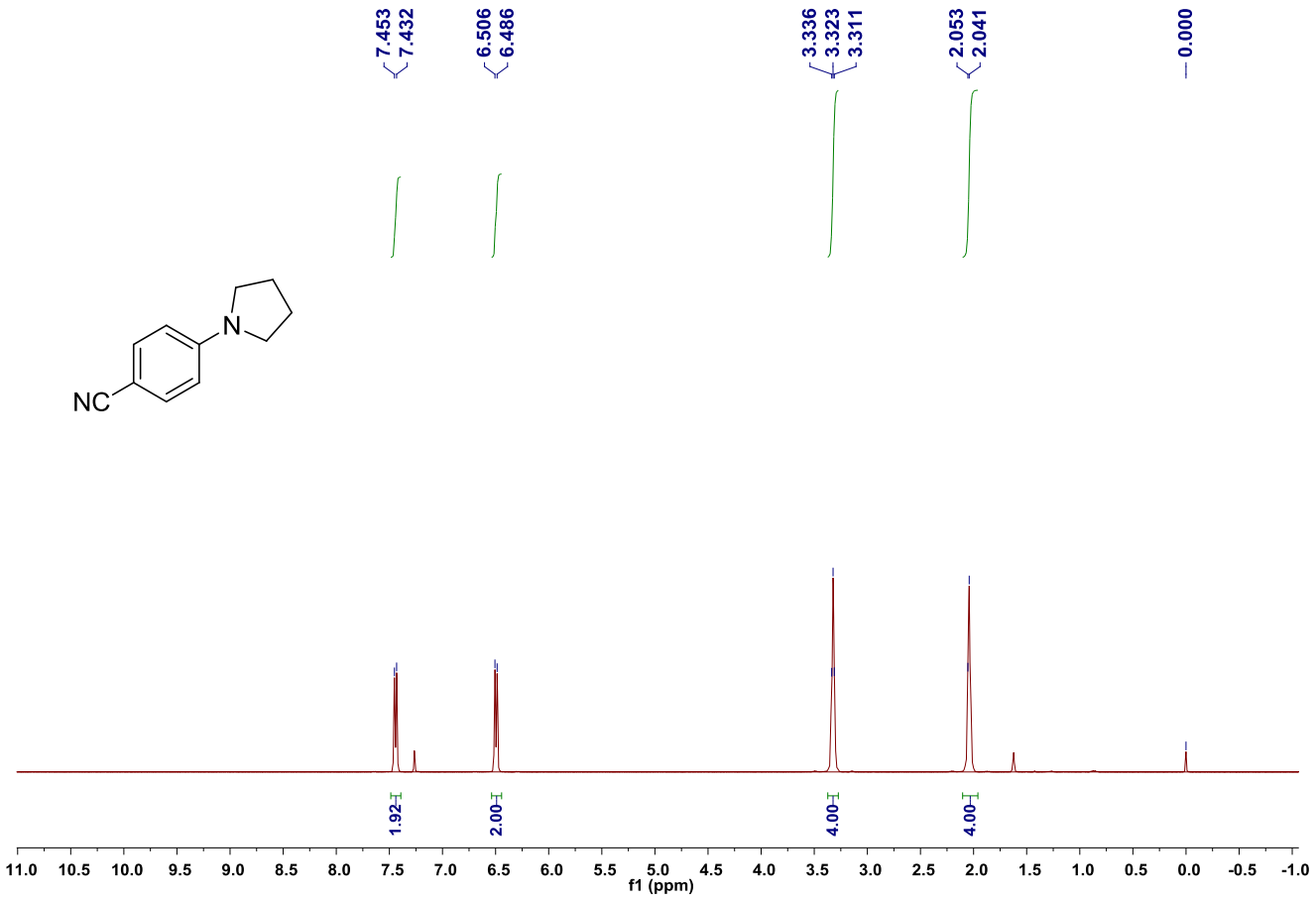
f1 (ppm)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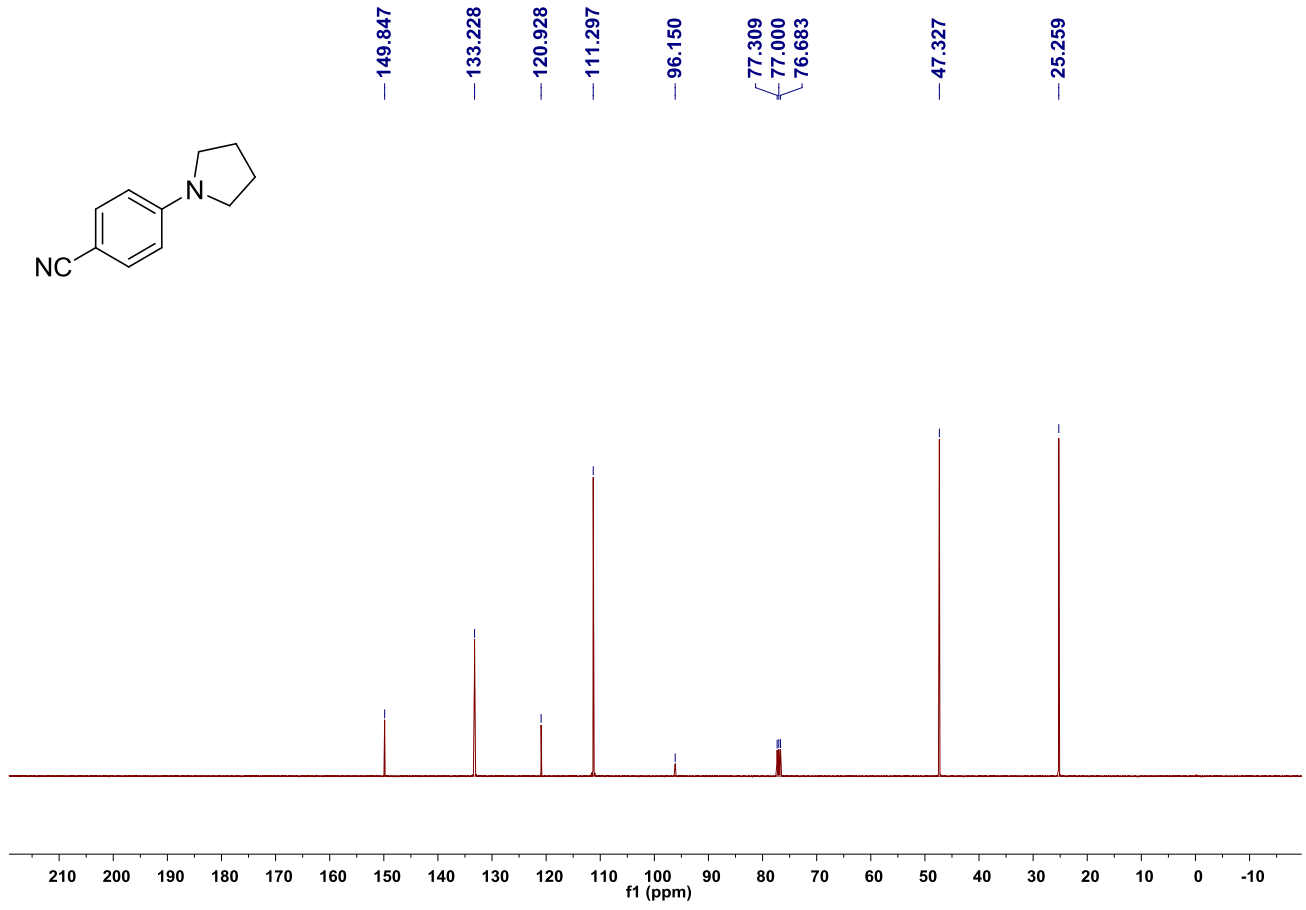
7.432
6.506
6.486
3.336
3.323
3.311
2.053
2.041
0.000
N
NC
1.92
2.00
4.00
4.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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77.309
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25.259
N
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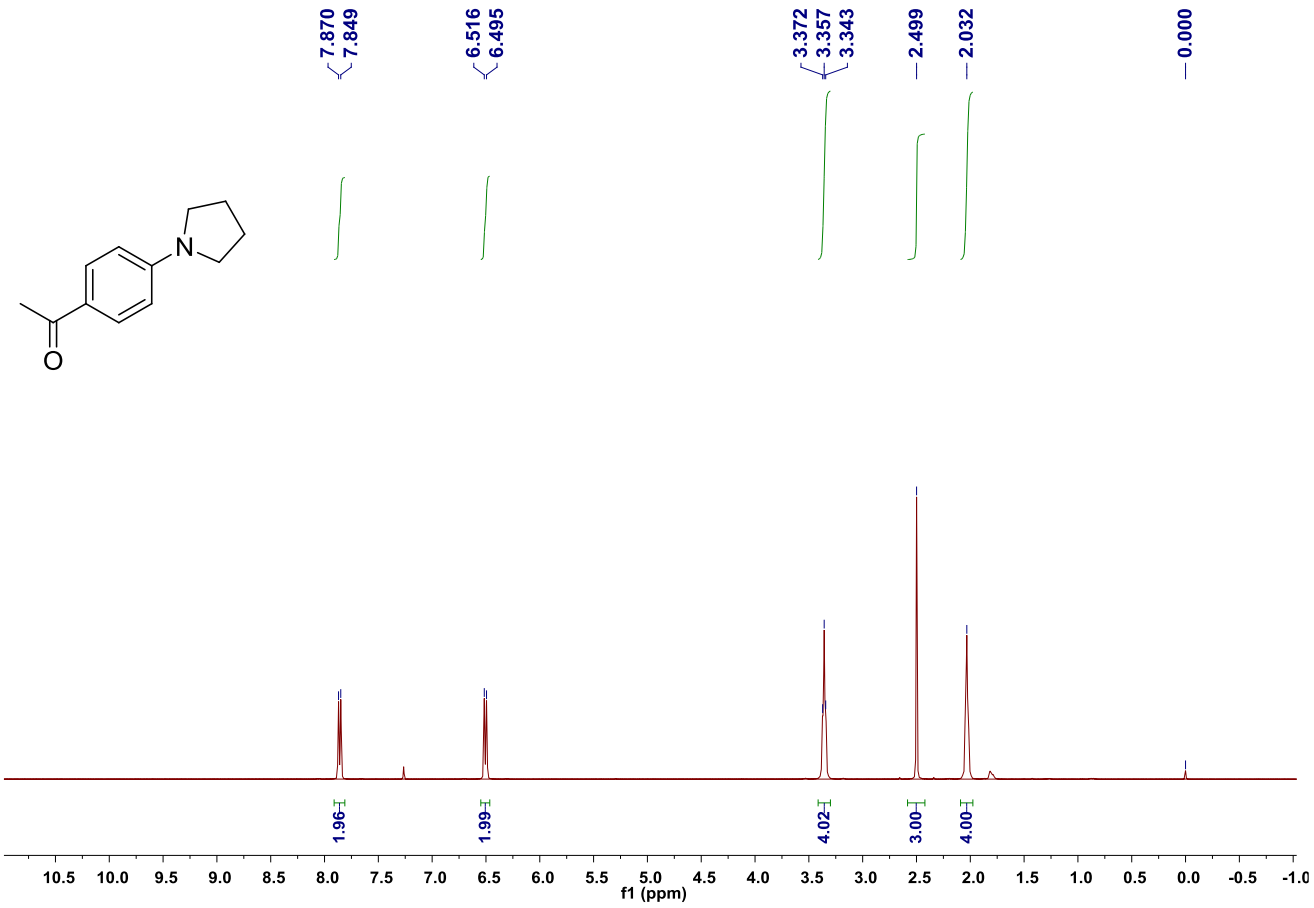
f1 (ppm)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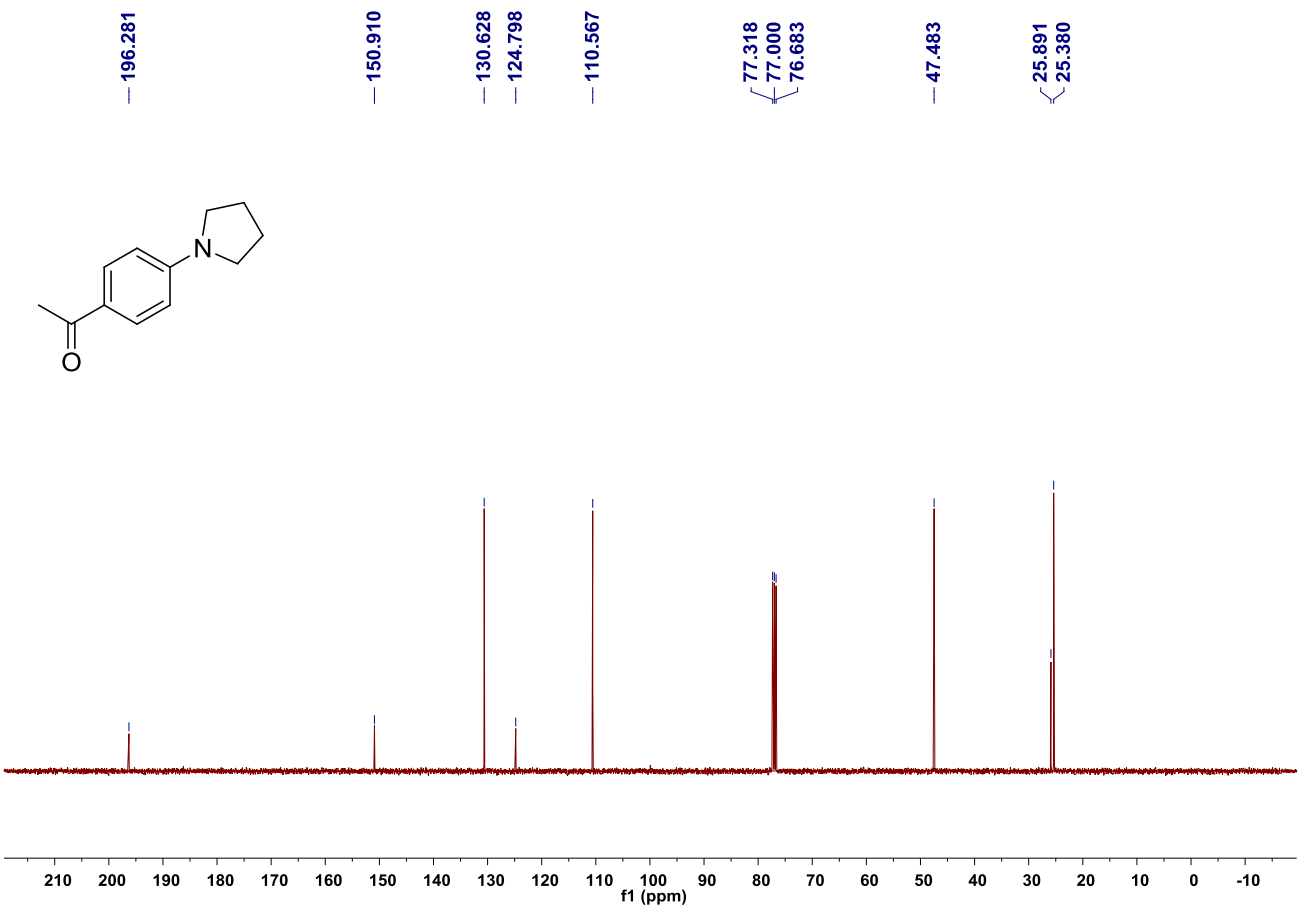
2.499
2.032
0.000
1.96
1.99
4.02
3.00
4.00
f1 (ppm)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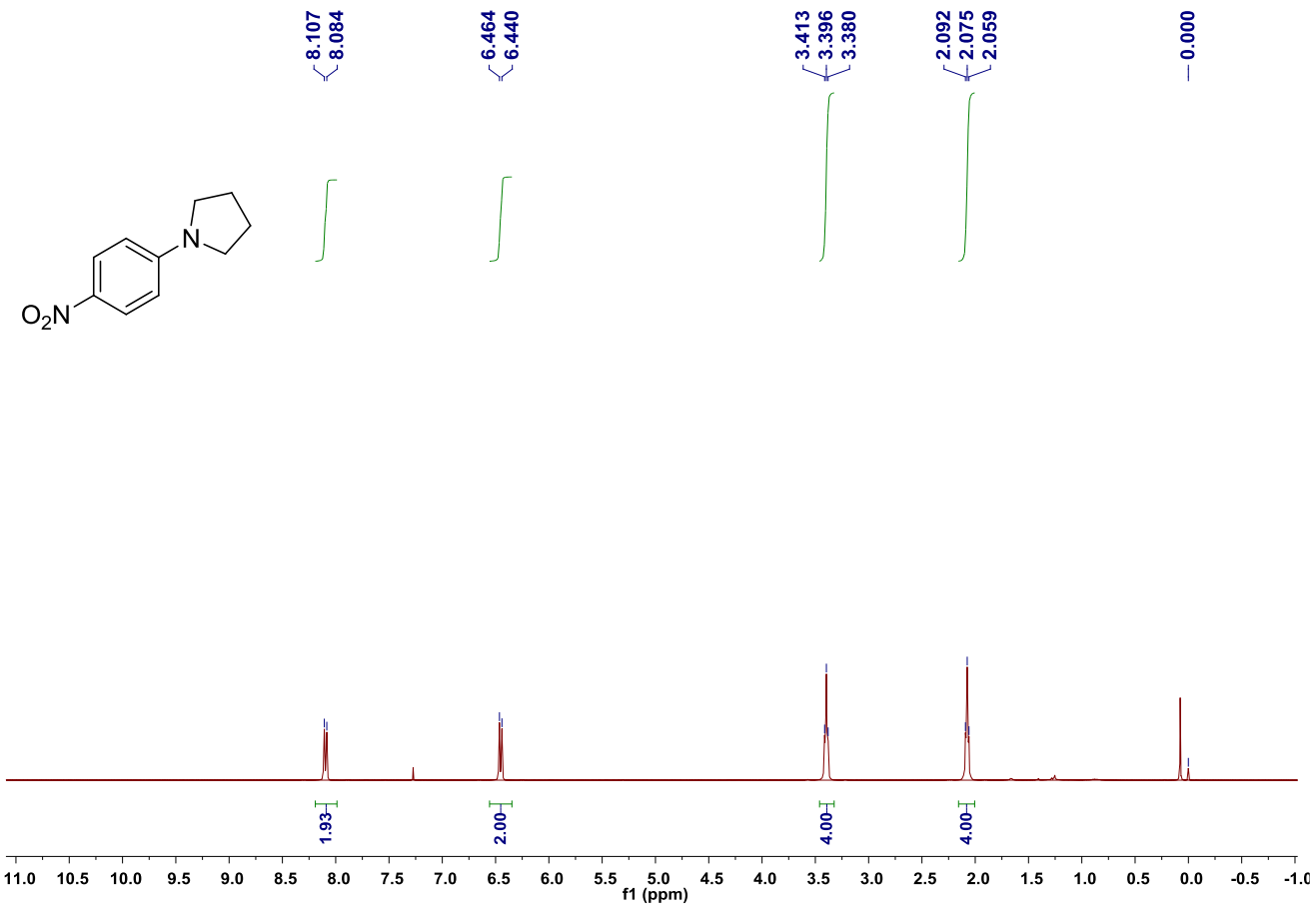
25.380
f1 (ppm)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6.440
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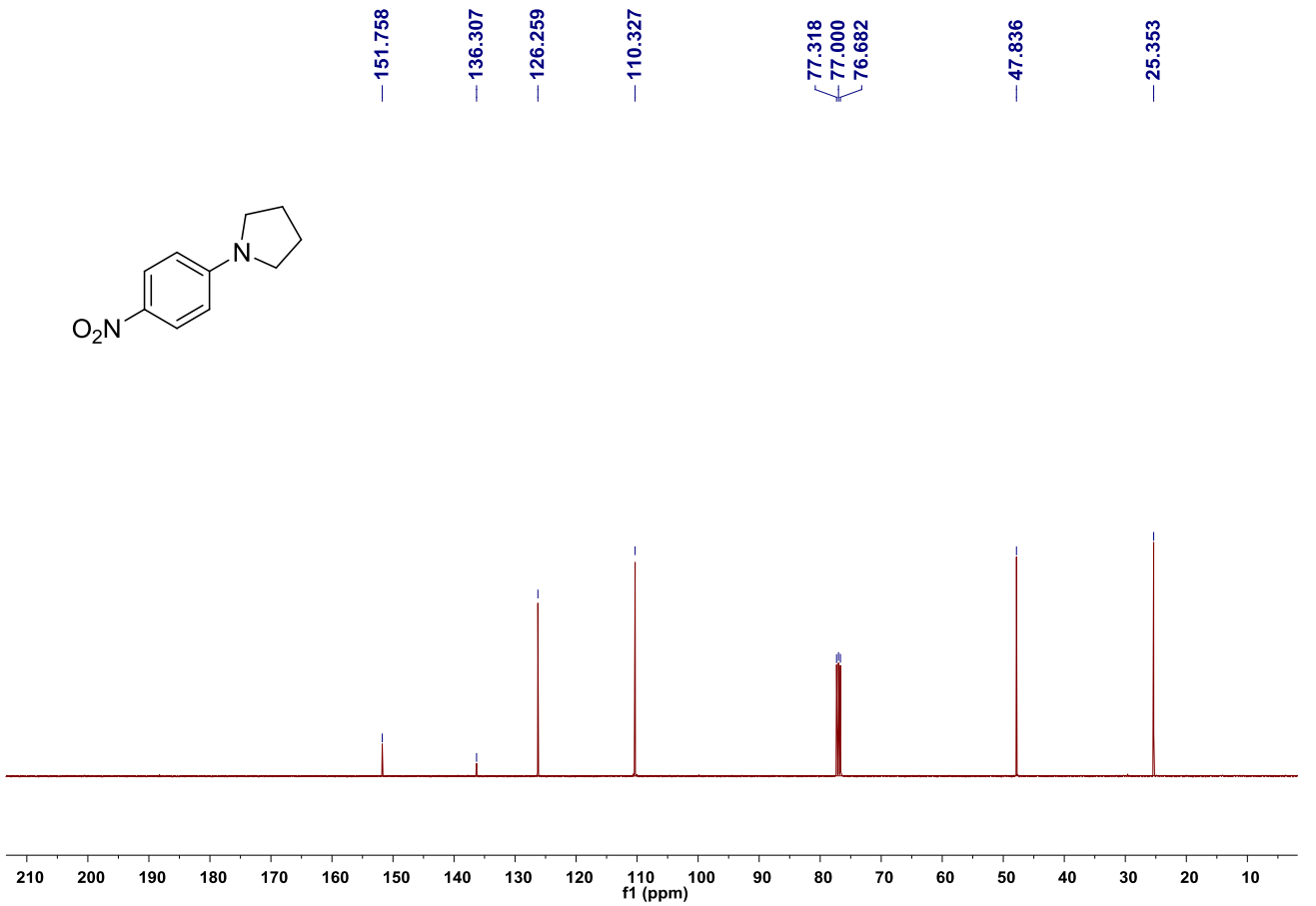
3.396
3.380
2.092
2.075
2.059
0.000
N
O2N
1.93
2.00
4.00
4.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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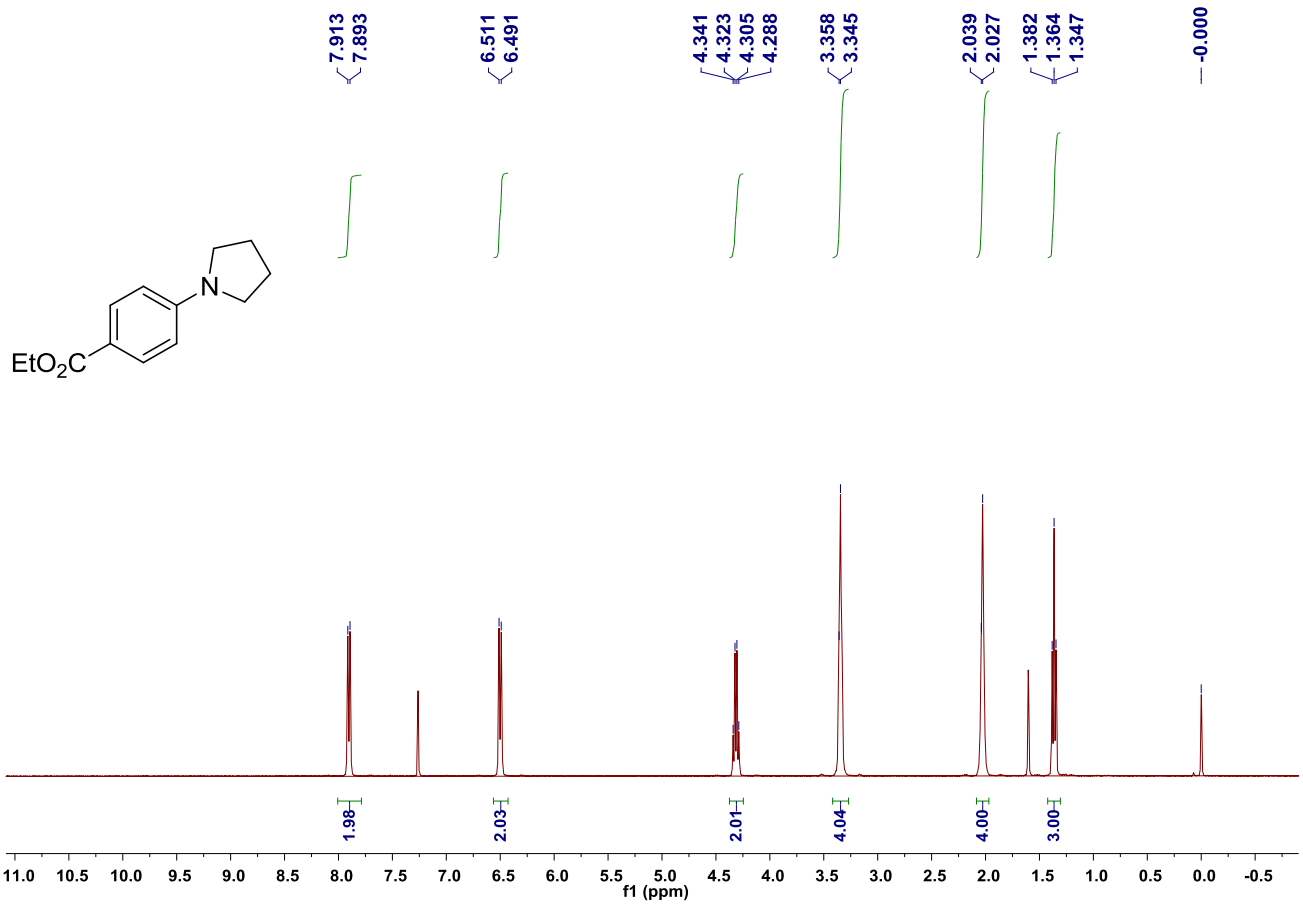
f1 (ppm)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2.027
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1.347
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N
EtO2C
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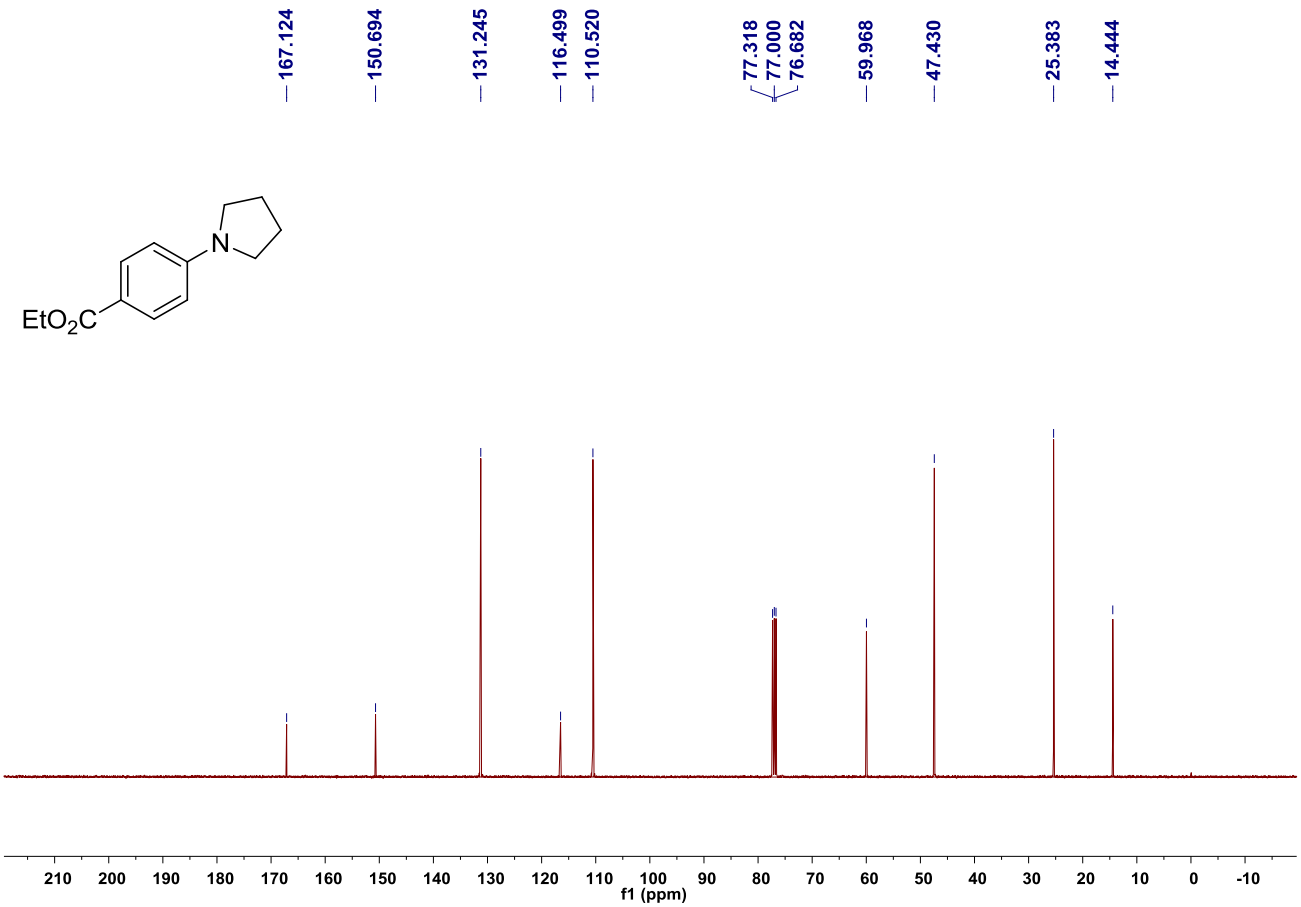
2.03
2.01
4.04
4.00
3.00
f1 (ppm)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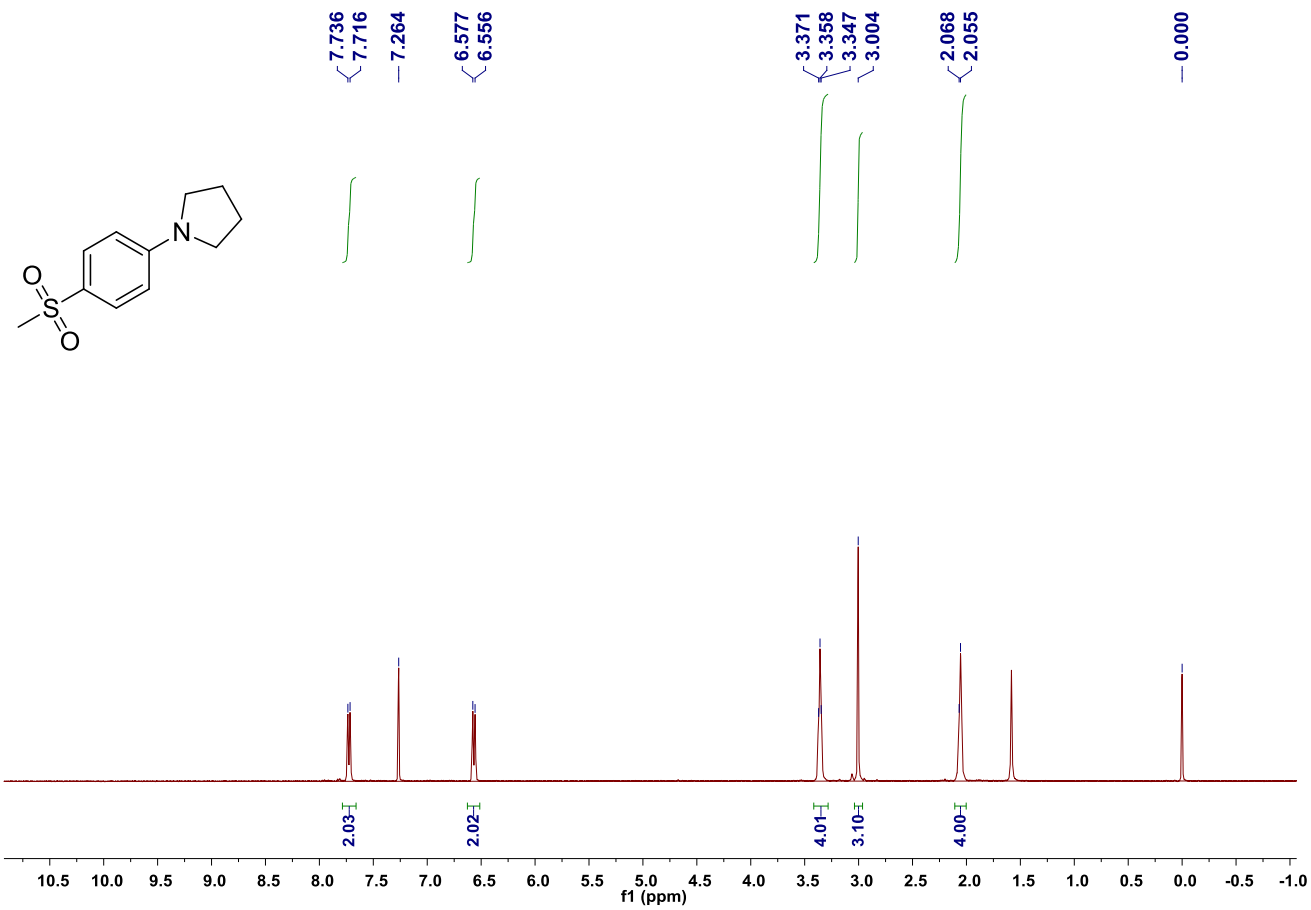
EtO2C
f1 (ppm)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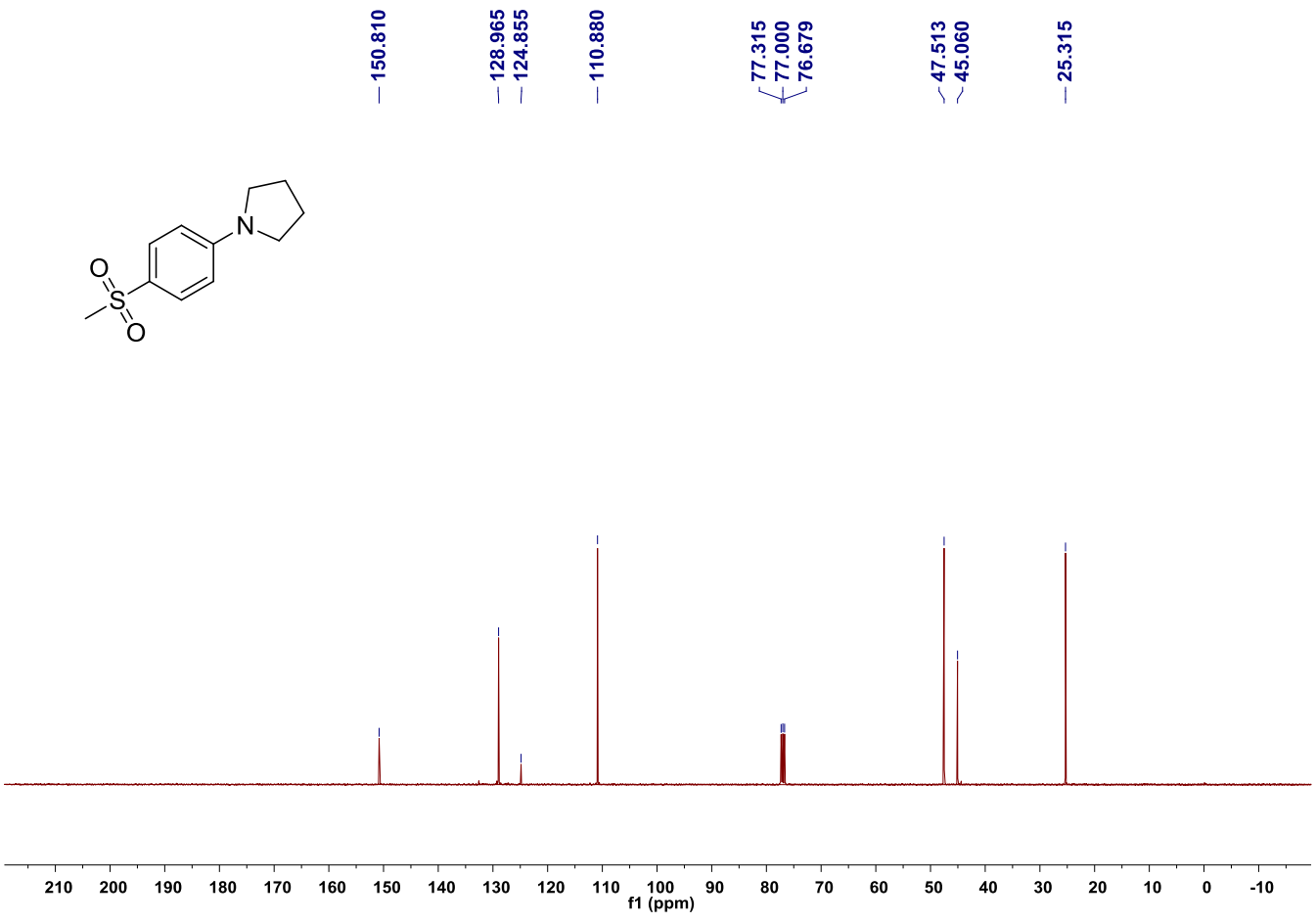
2.02
4.01
3.10
4.00
f1 (ppm)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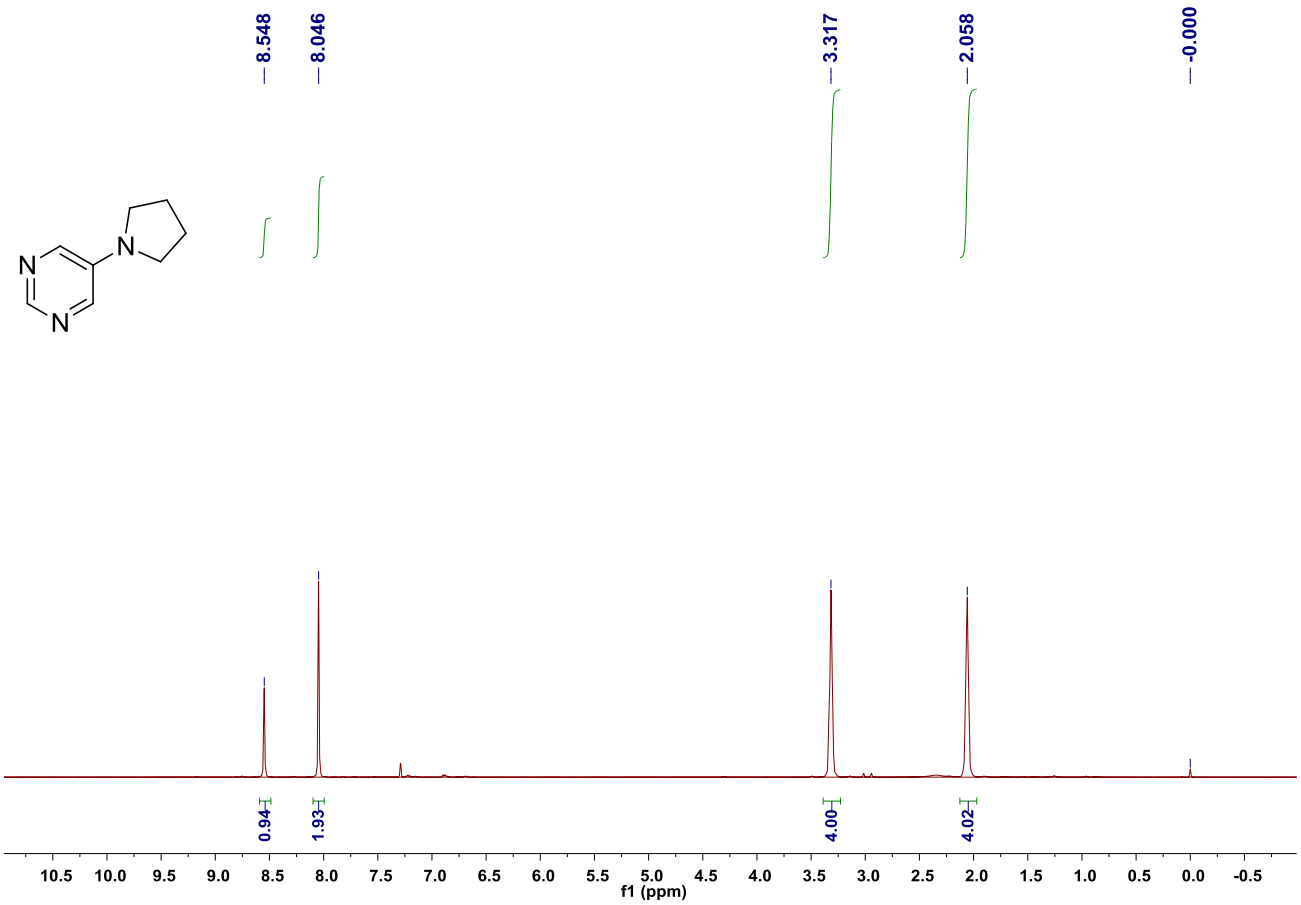
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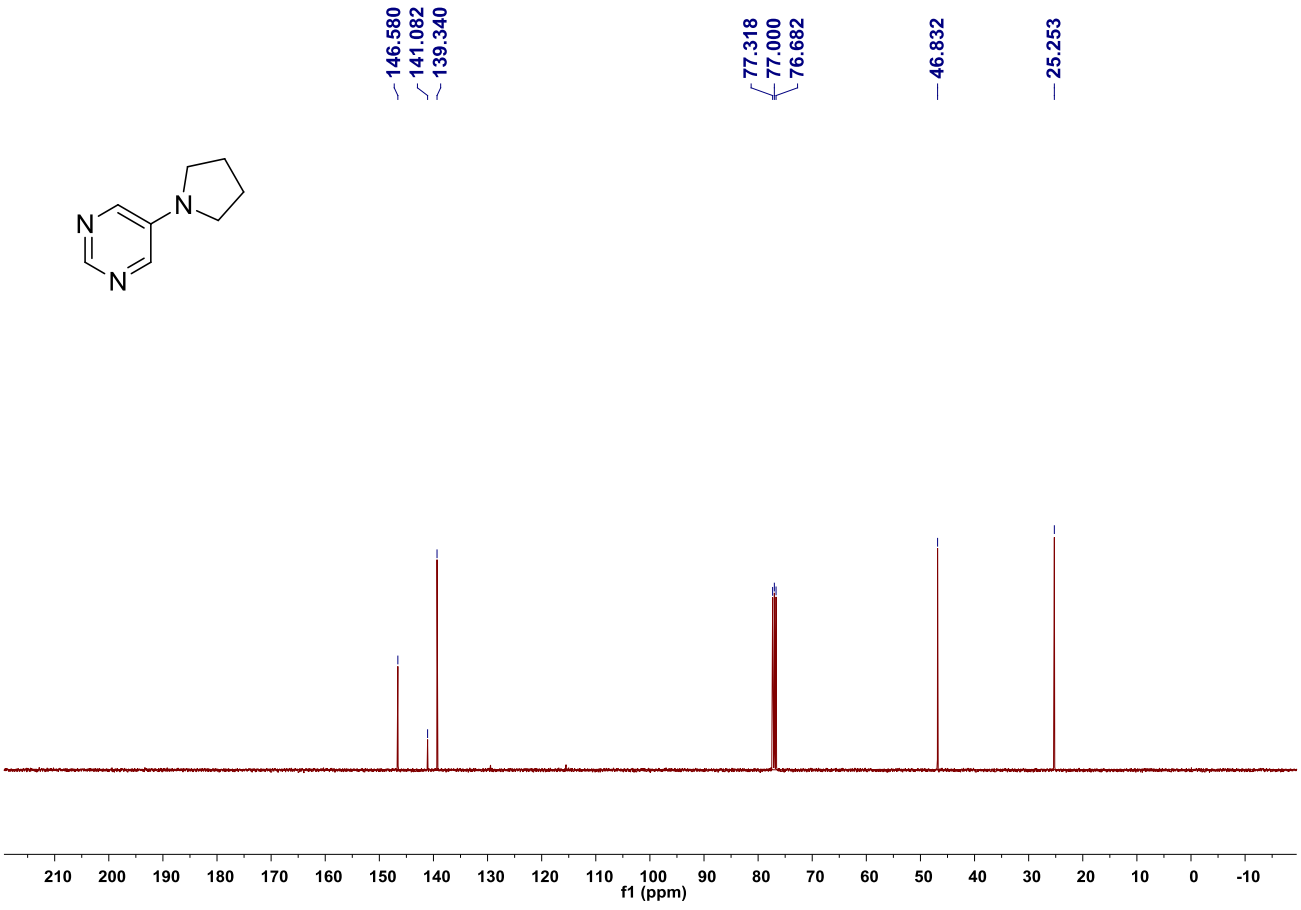
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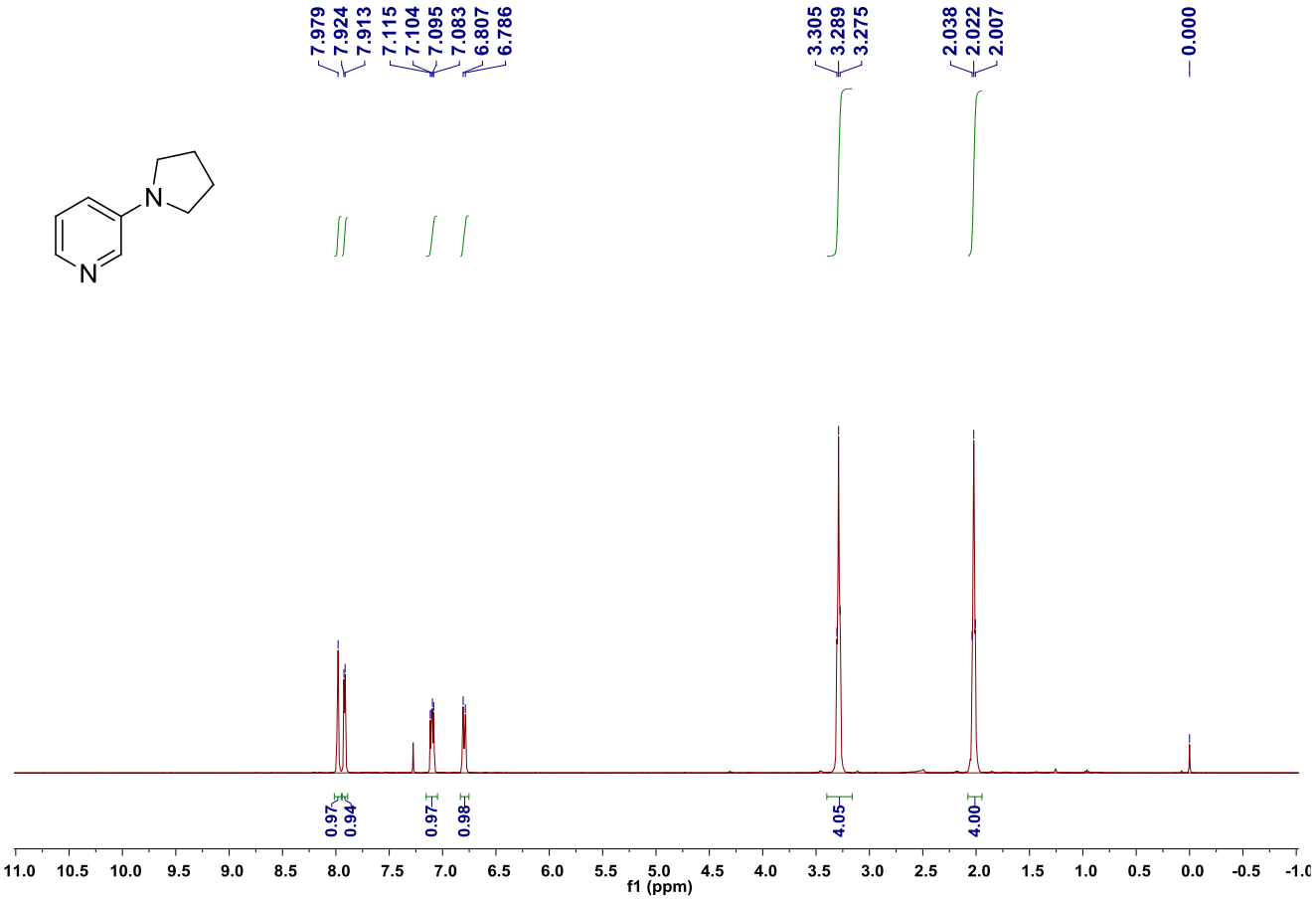
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7.104
7.095
7.083
6.807
6.786
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2.007
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0.97
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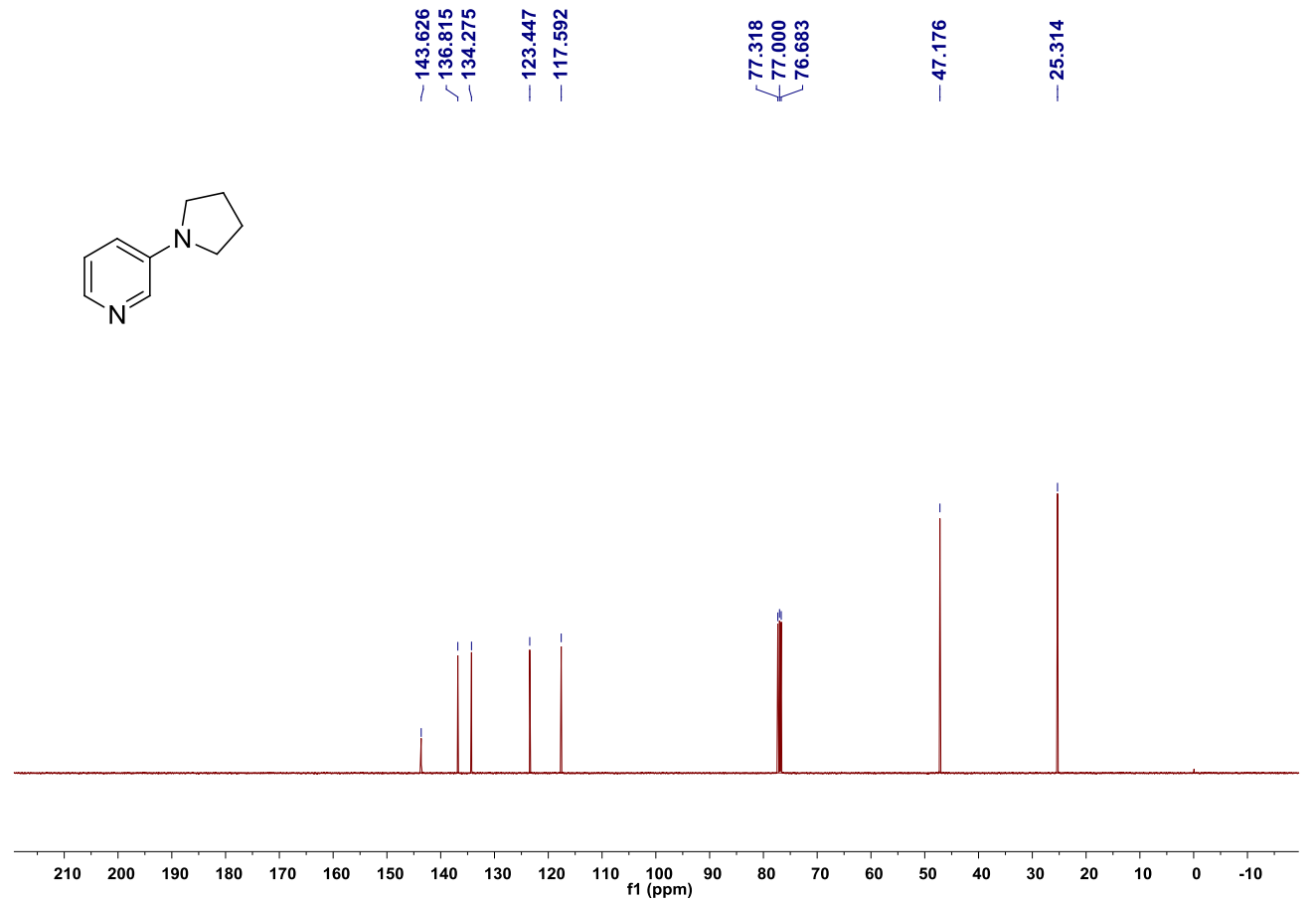
f1 (ppm)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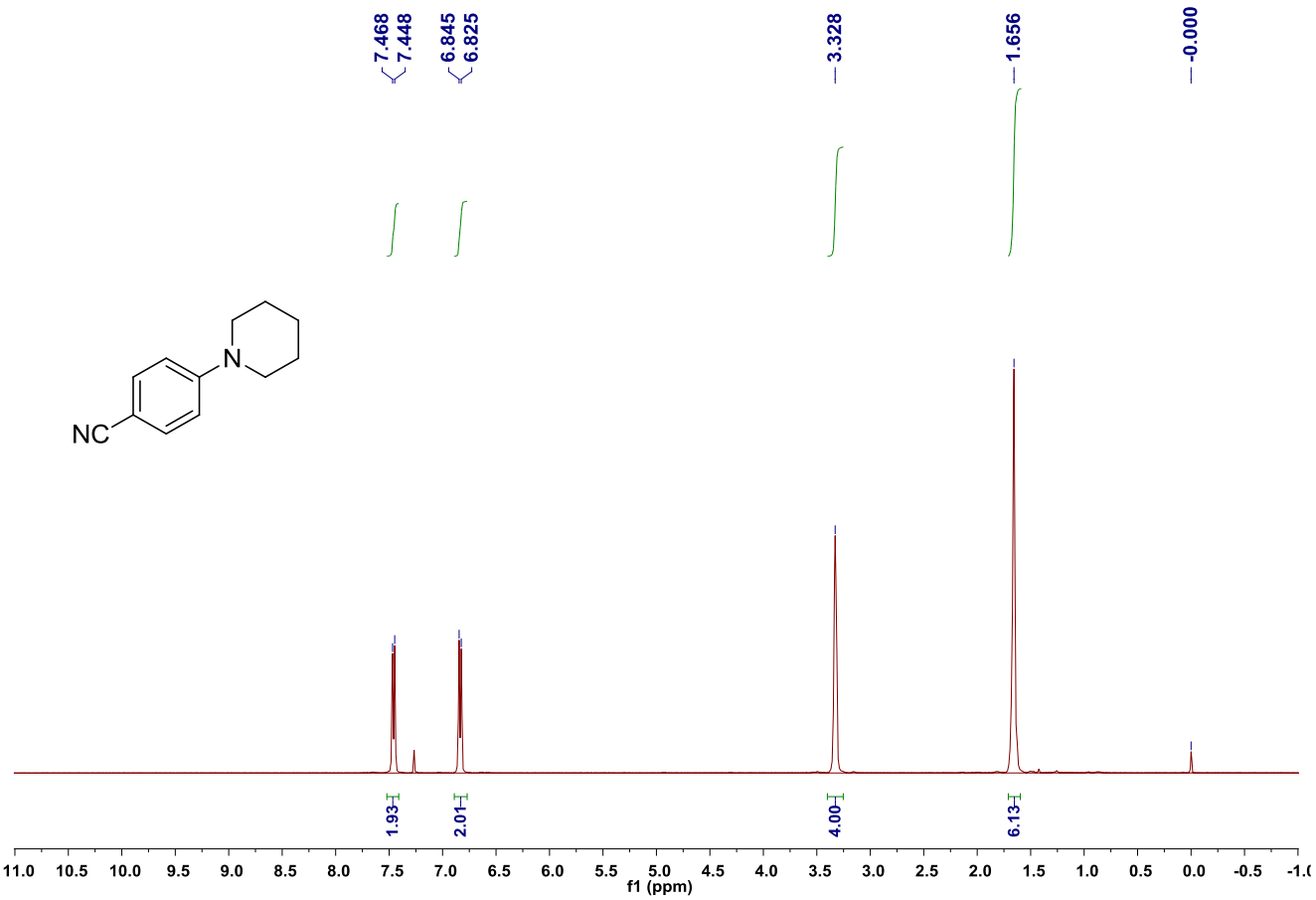
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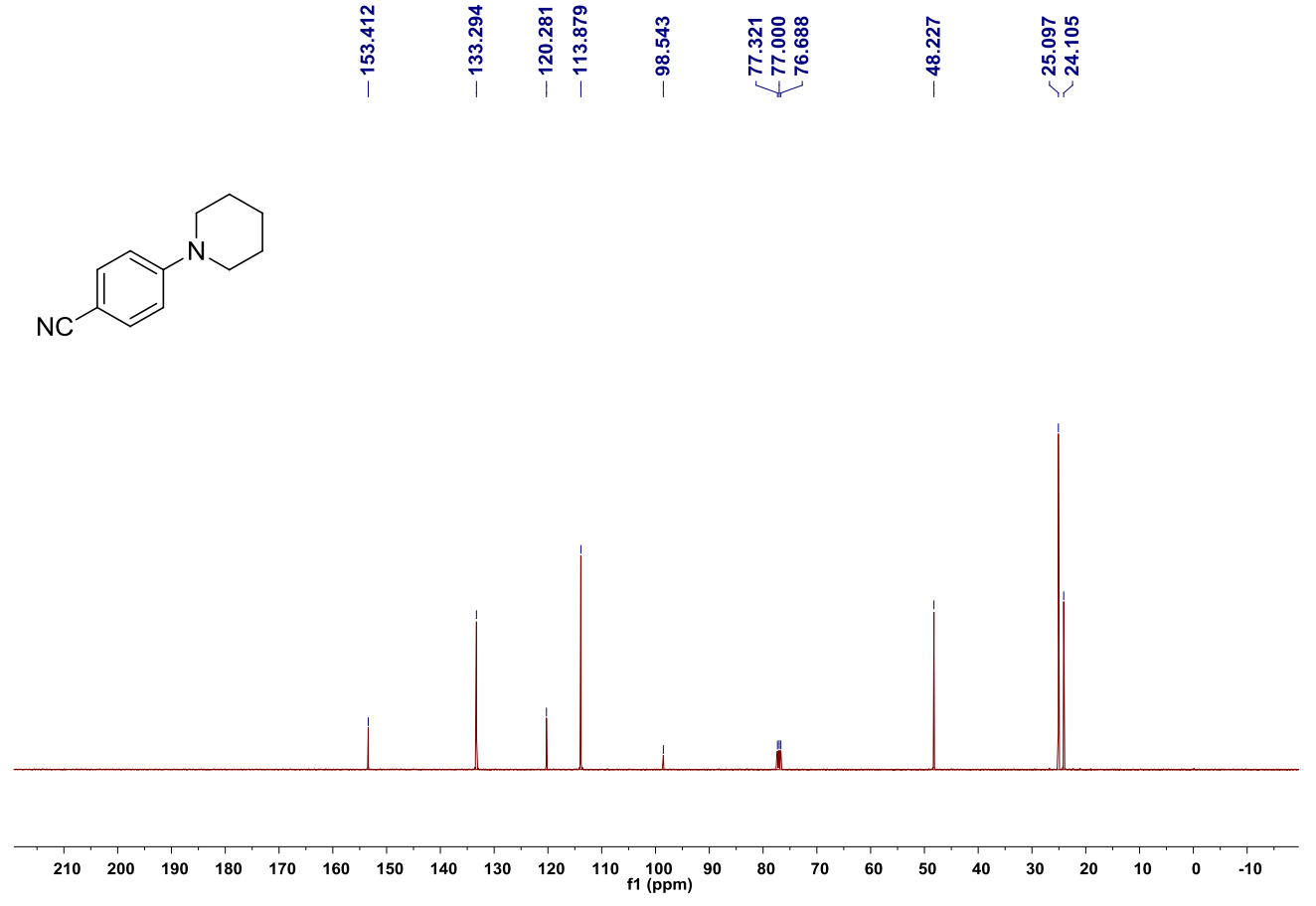
f1 (ppm)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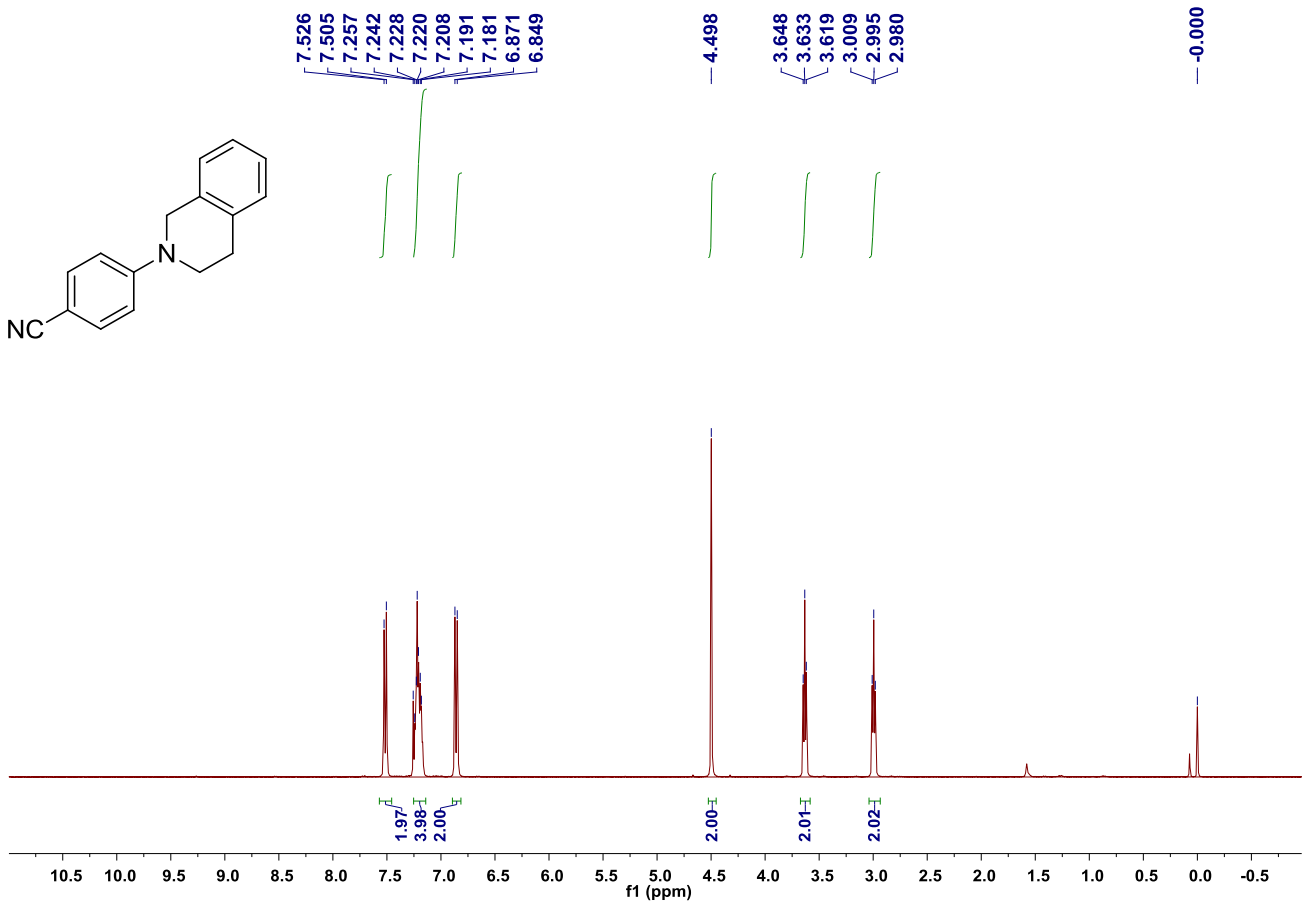
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3.648
3.633
3.619
3.009
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2.00
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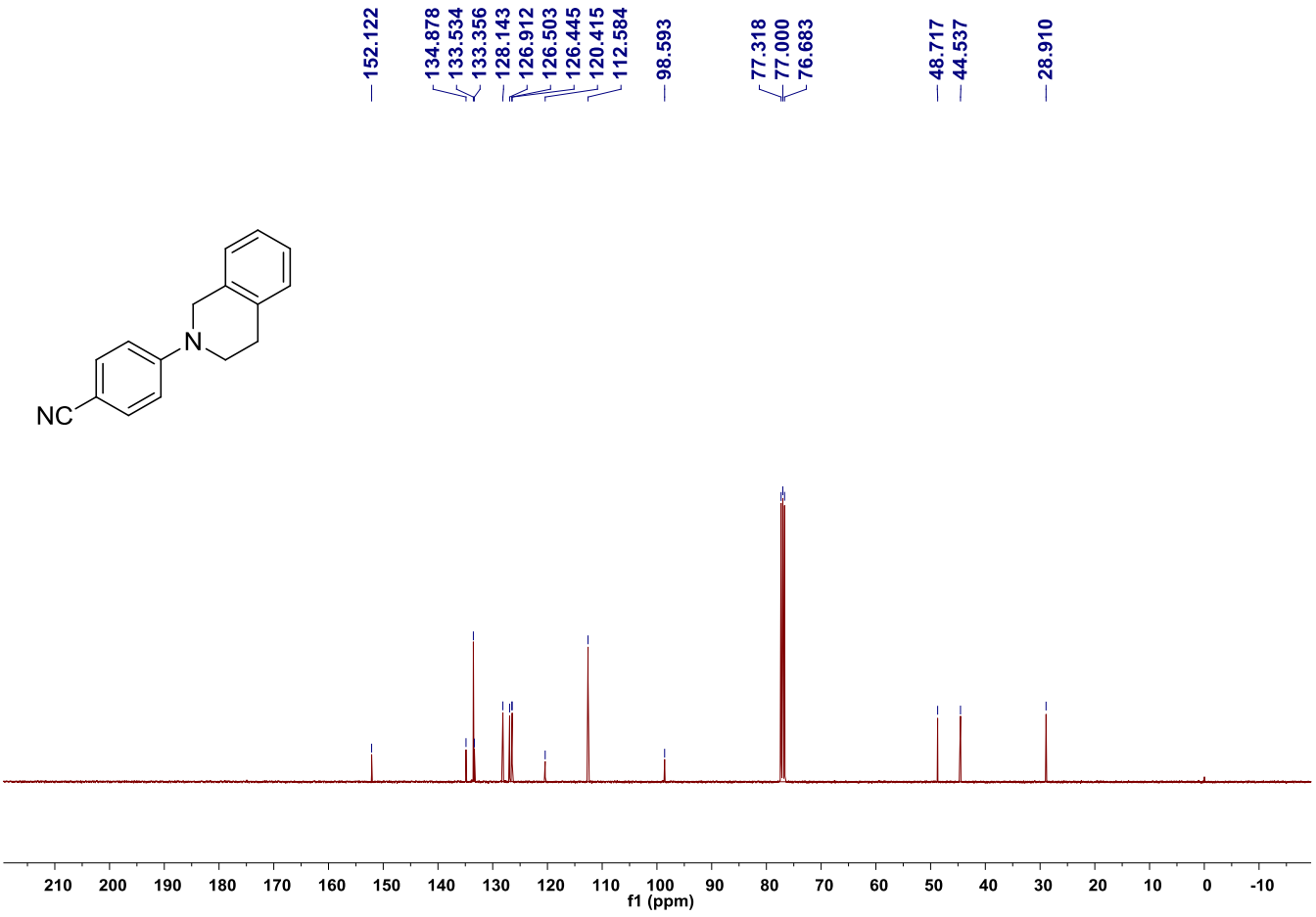
2.02
f1 (ppm)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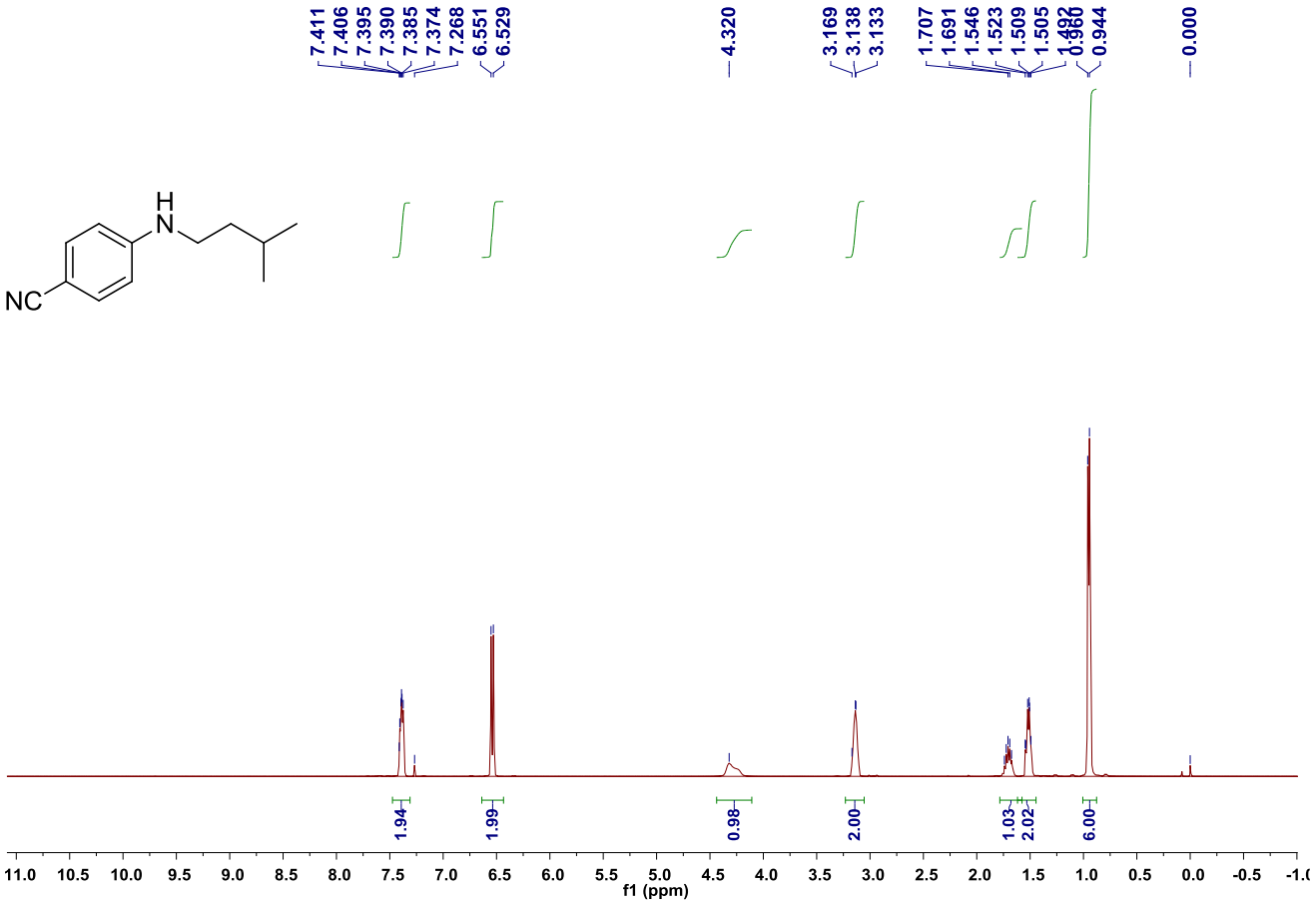
f1 (ppm)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3.133
1.707
1.691
1.546
1.523
1.509
1.505
0.960
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H
N
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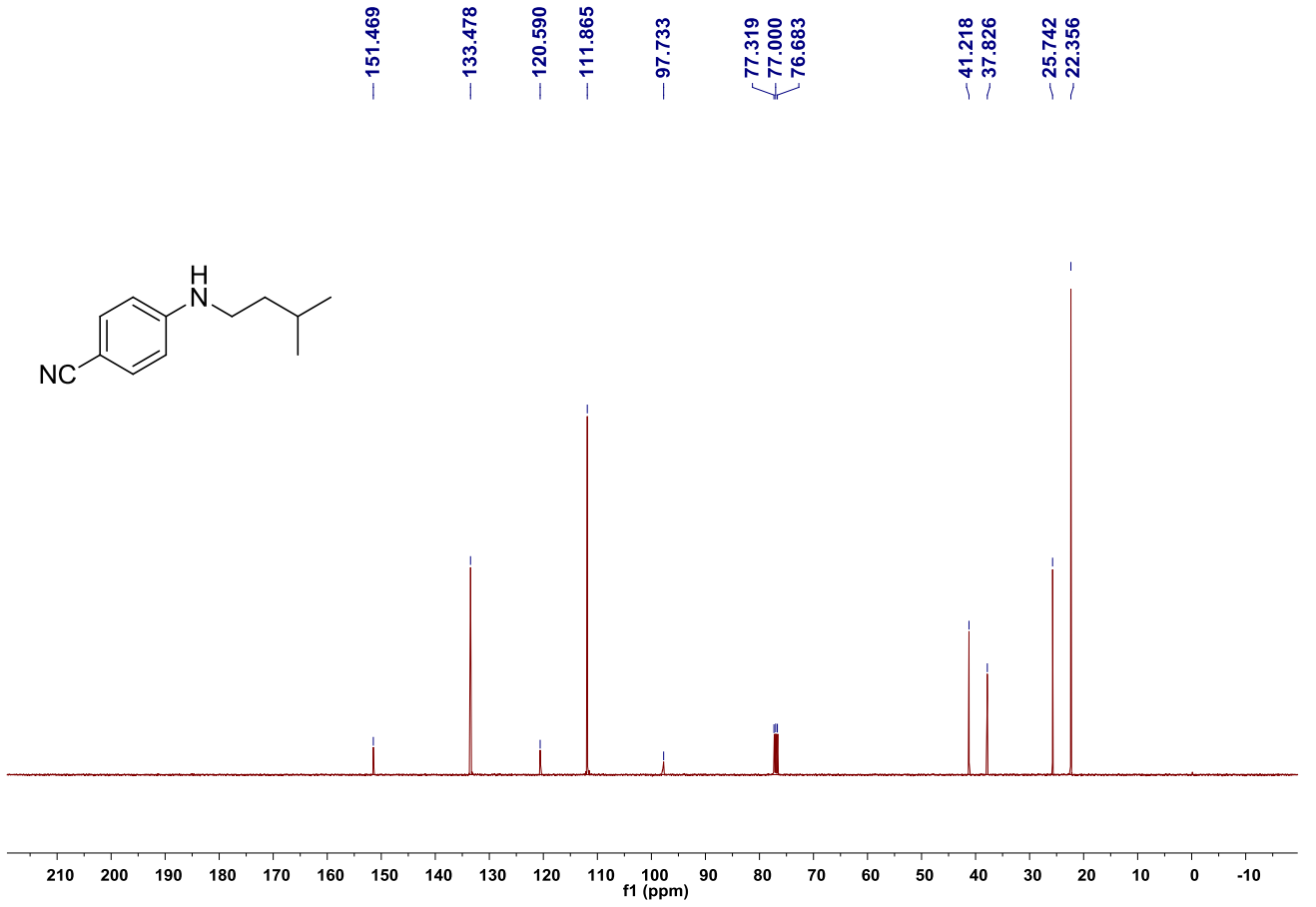
f1 (ppm)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N
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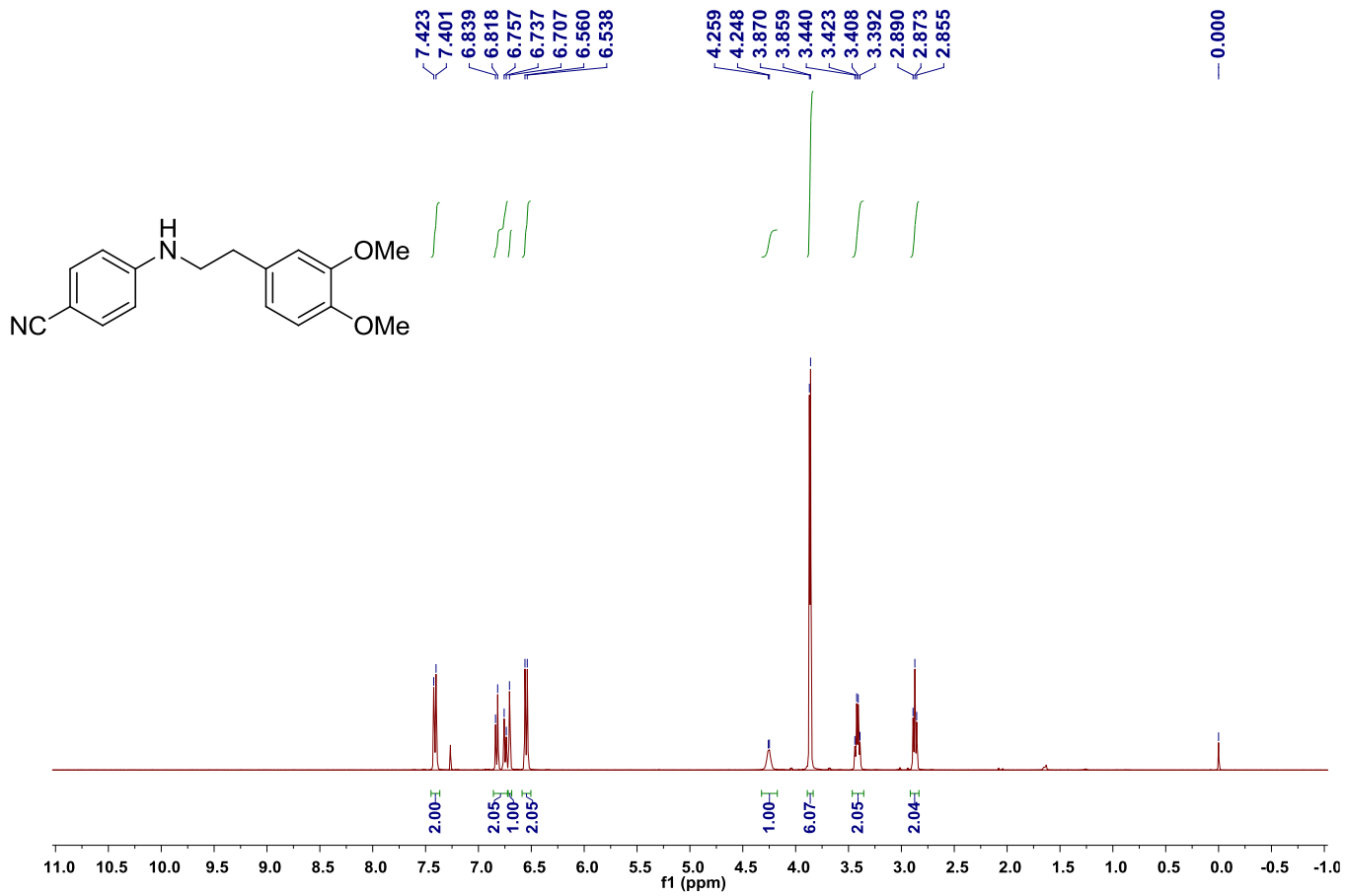
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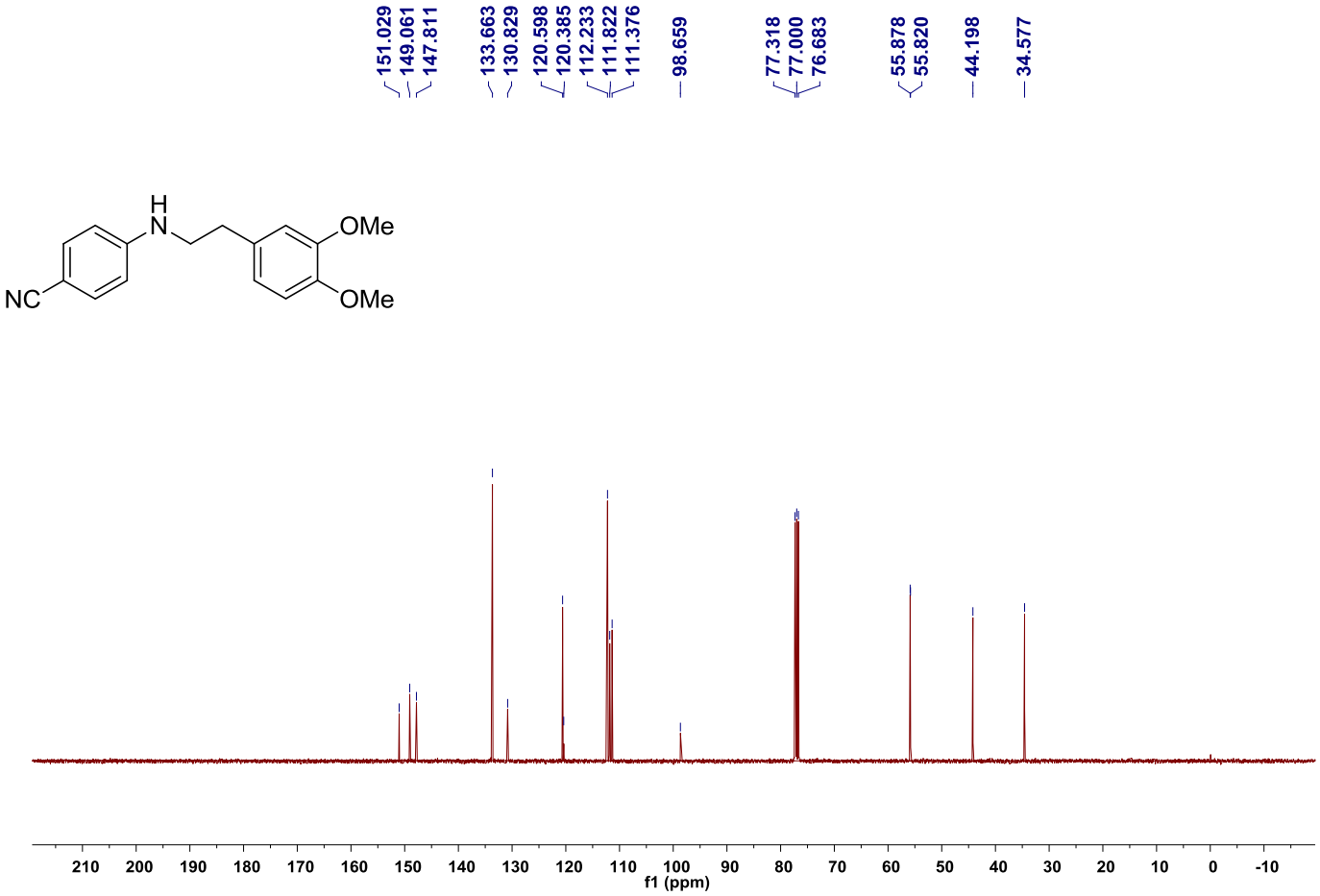
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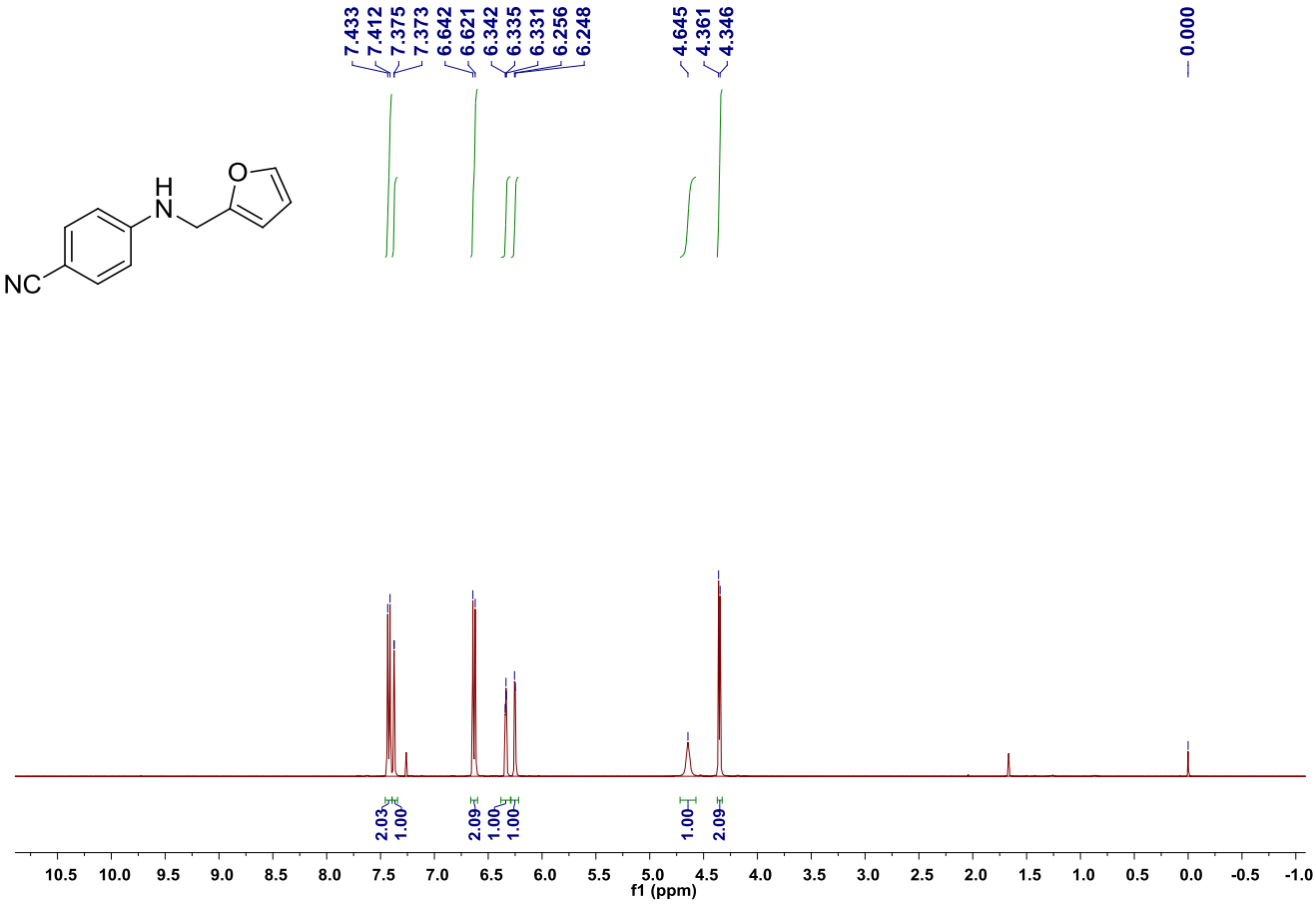
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H
N
O
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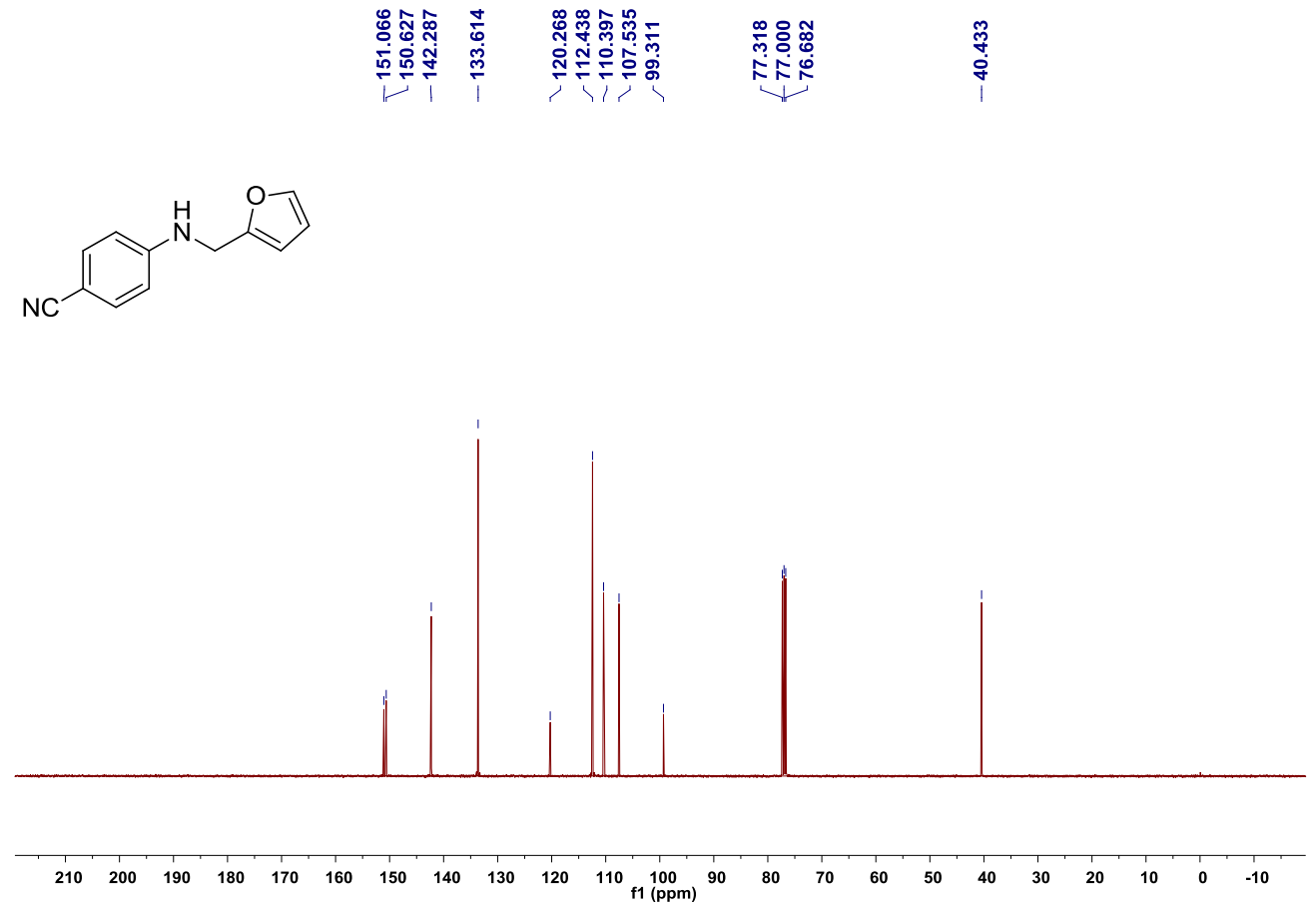
f1 (ppm)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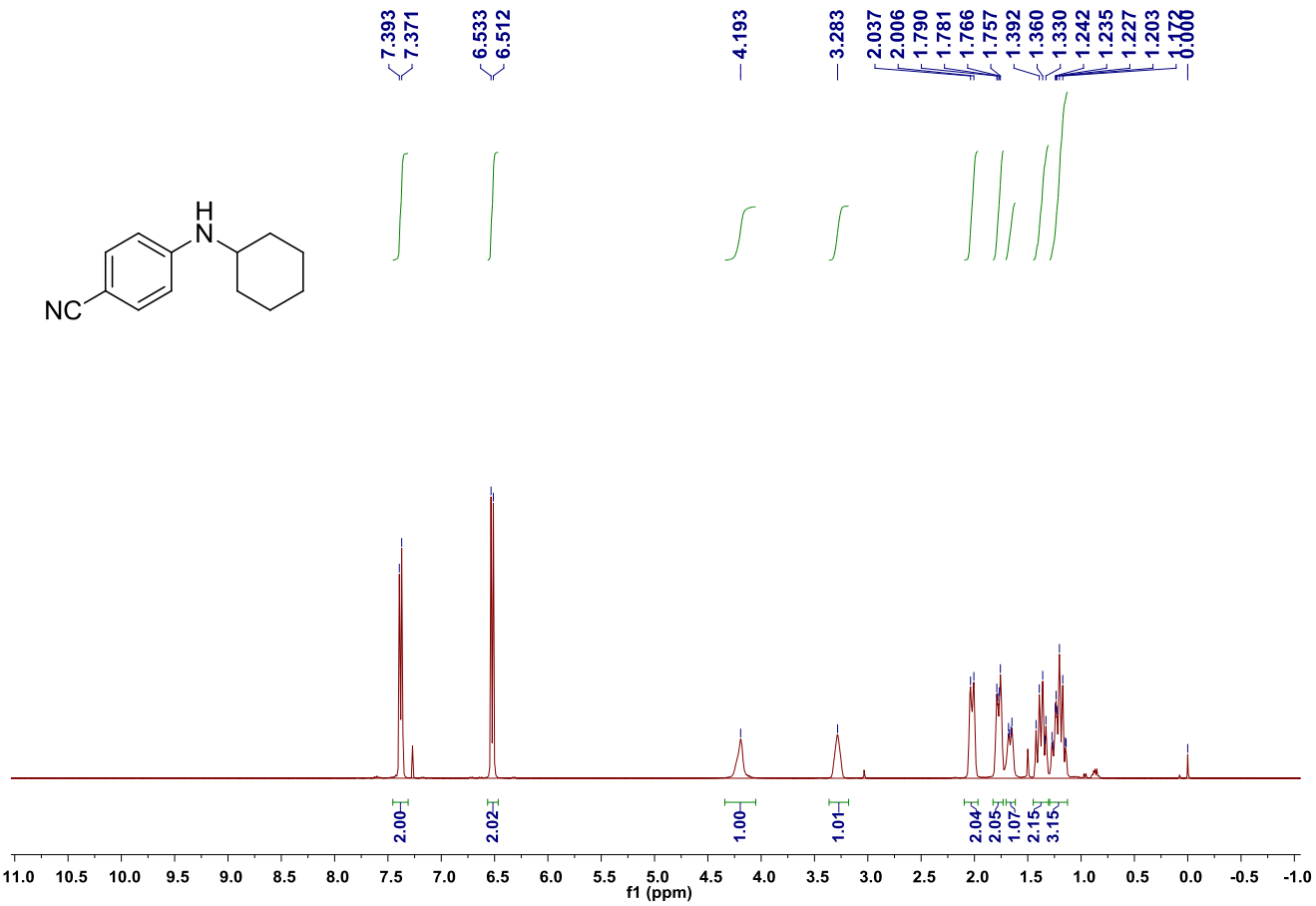
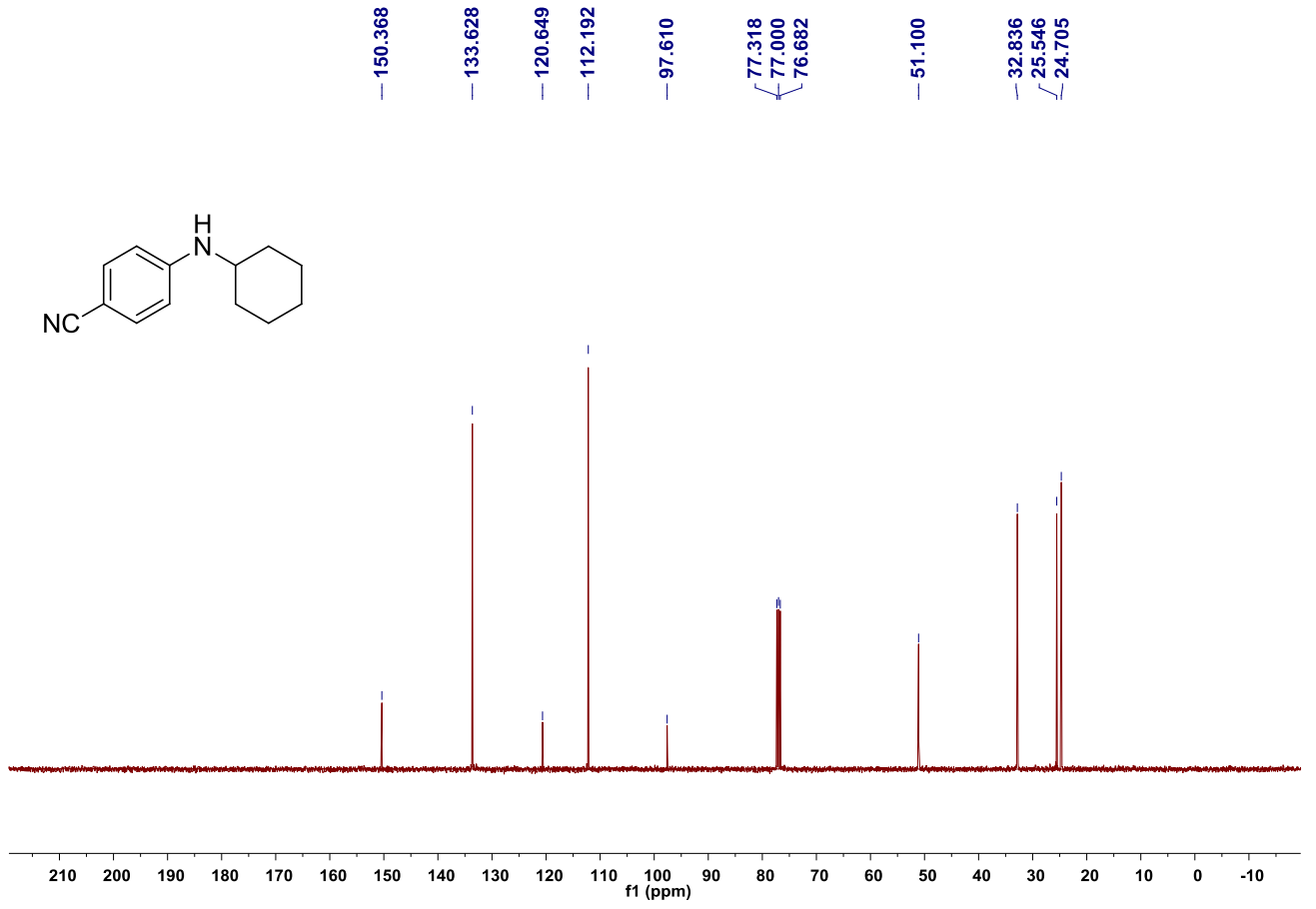
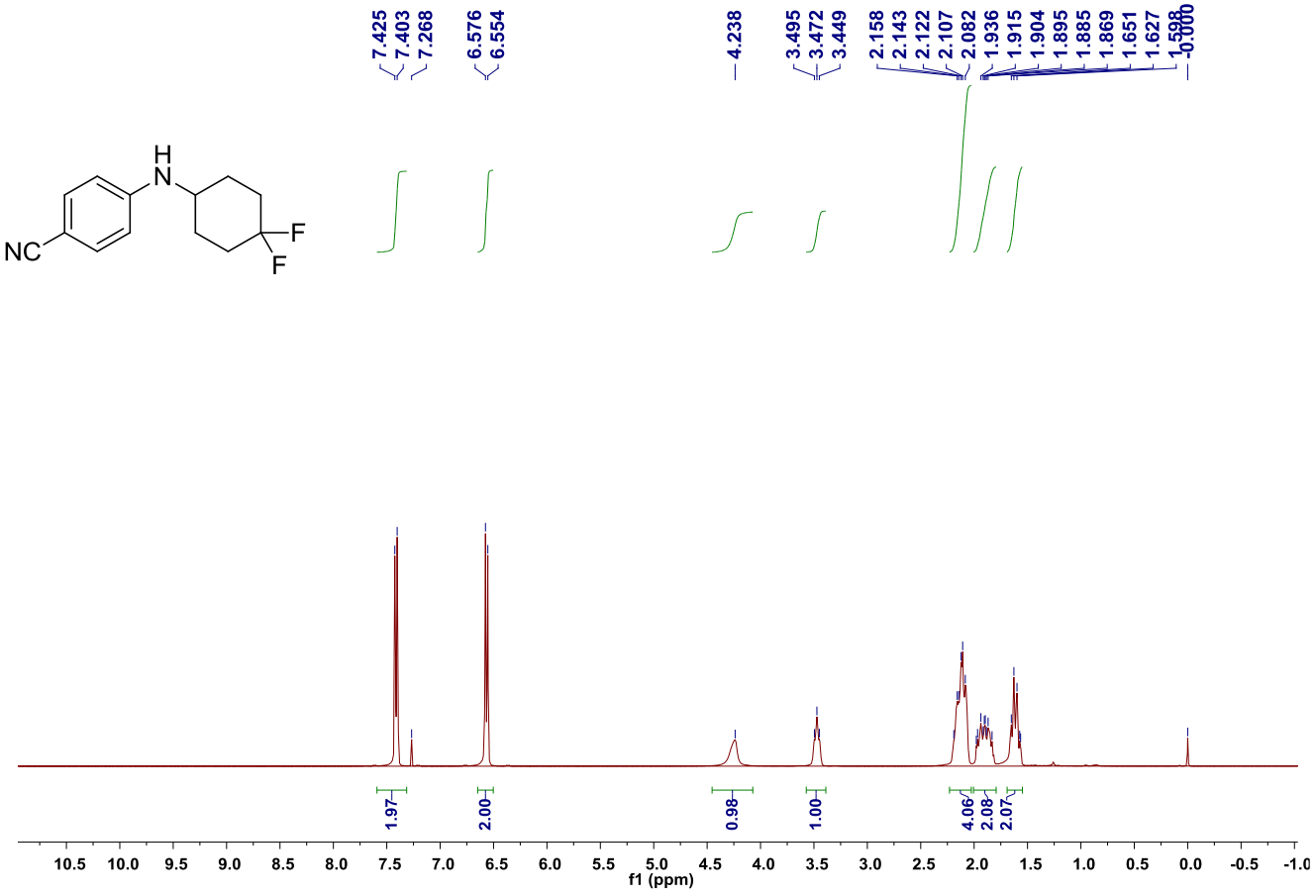
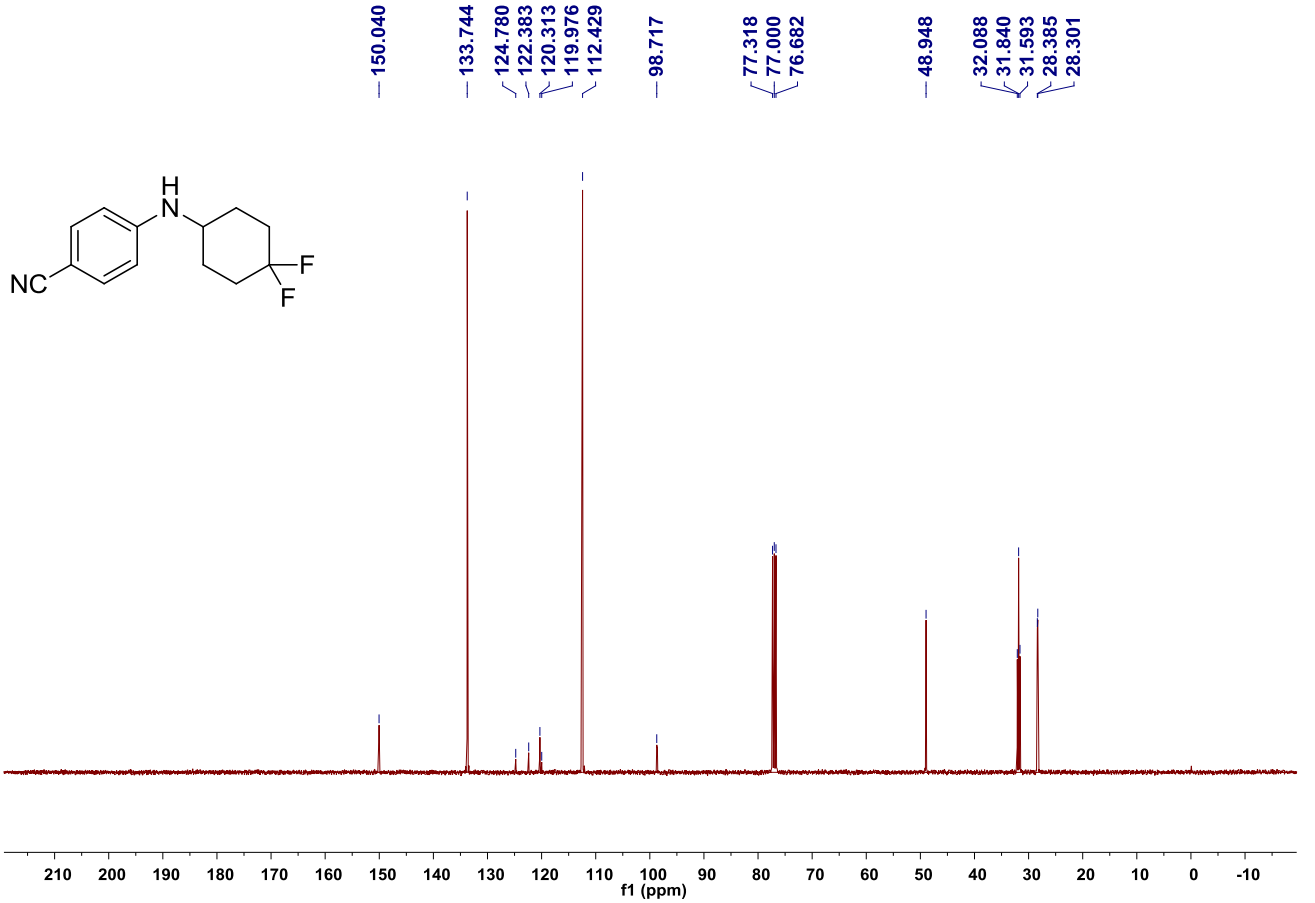
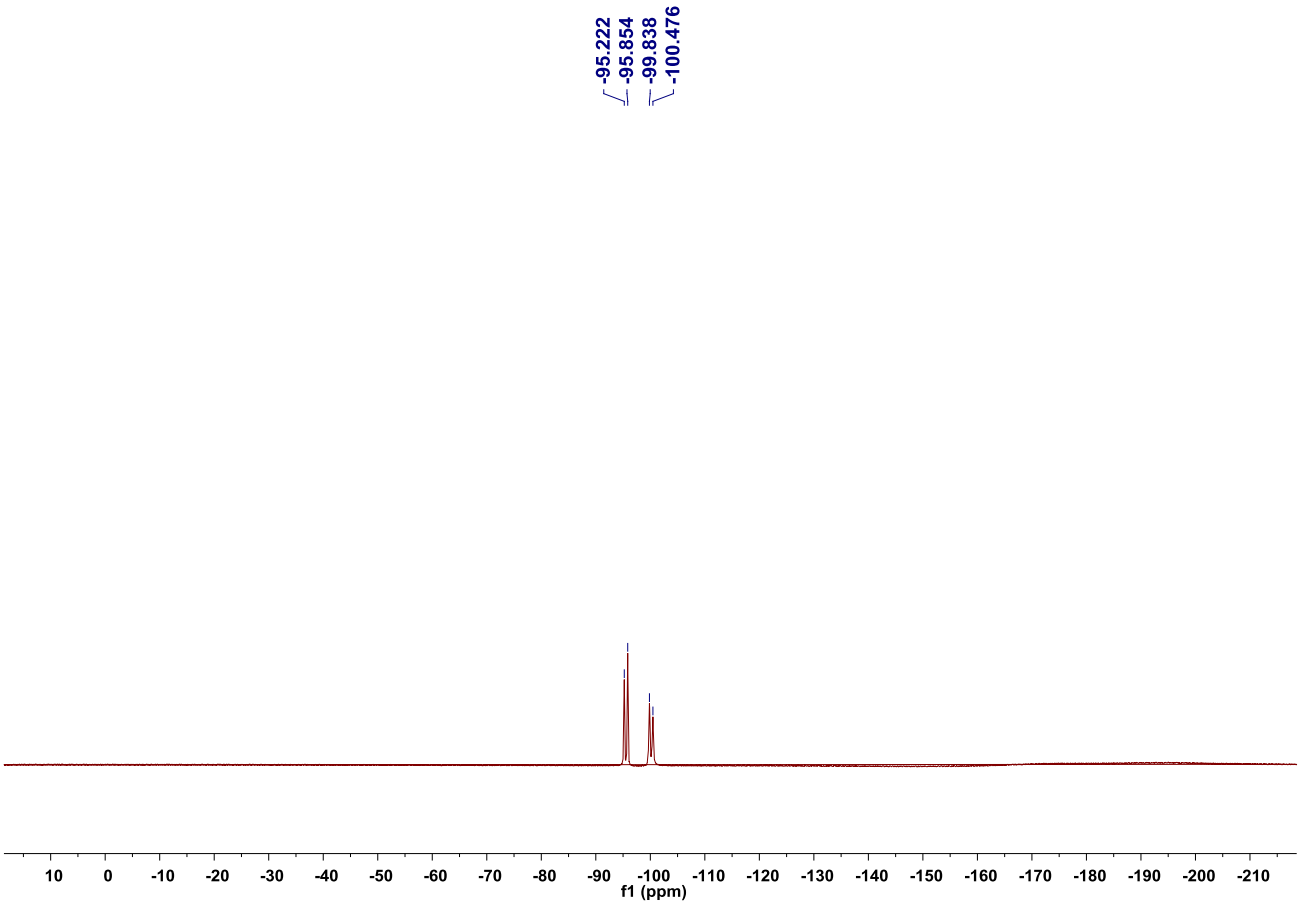
O
f1 (ppm)

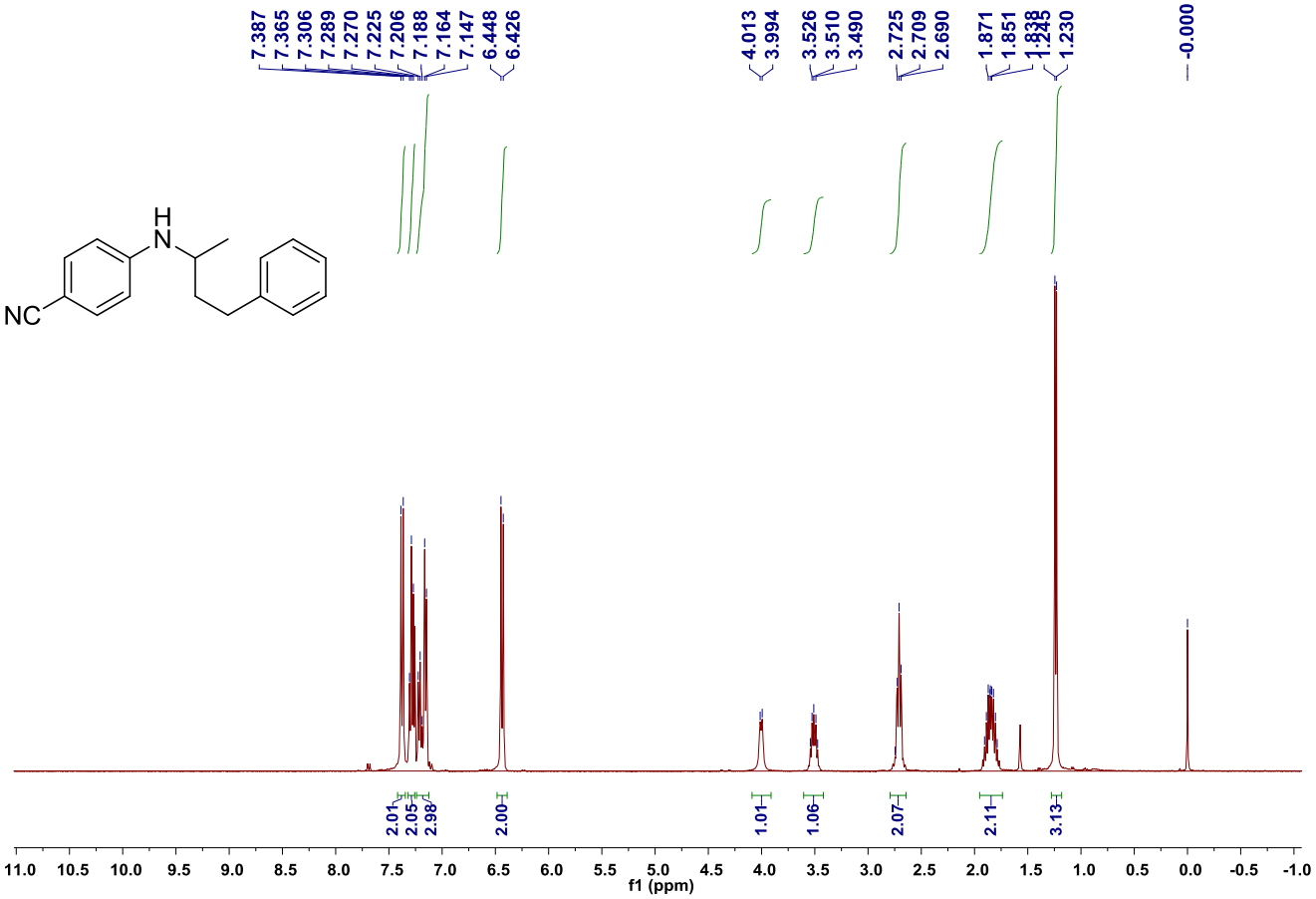

7.393
7.371
6.533
6.512
4.193
3.283
2.037
2.006
1.790
1.781
1.766
1.757
1.392
1.360
1.330
1.242
1.235
1.227
1.203
1.172
0.000
H
N
NC
2.00
2.02
1.00
1.01
2.04
2.05
1.07
2.15
3.15
f1 (ppm)

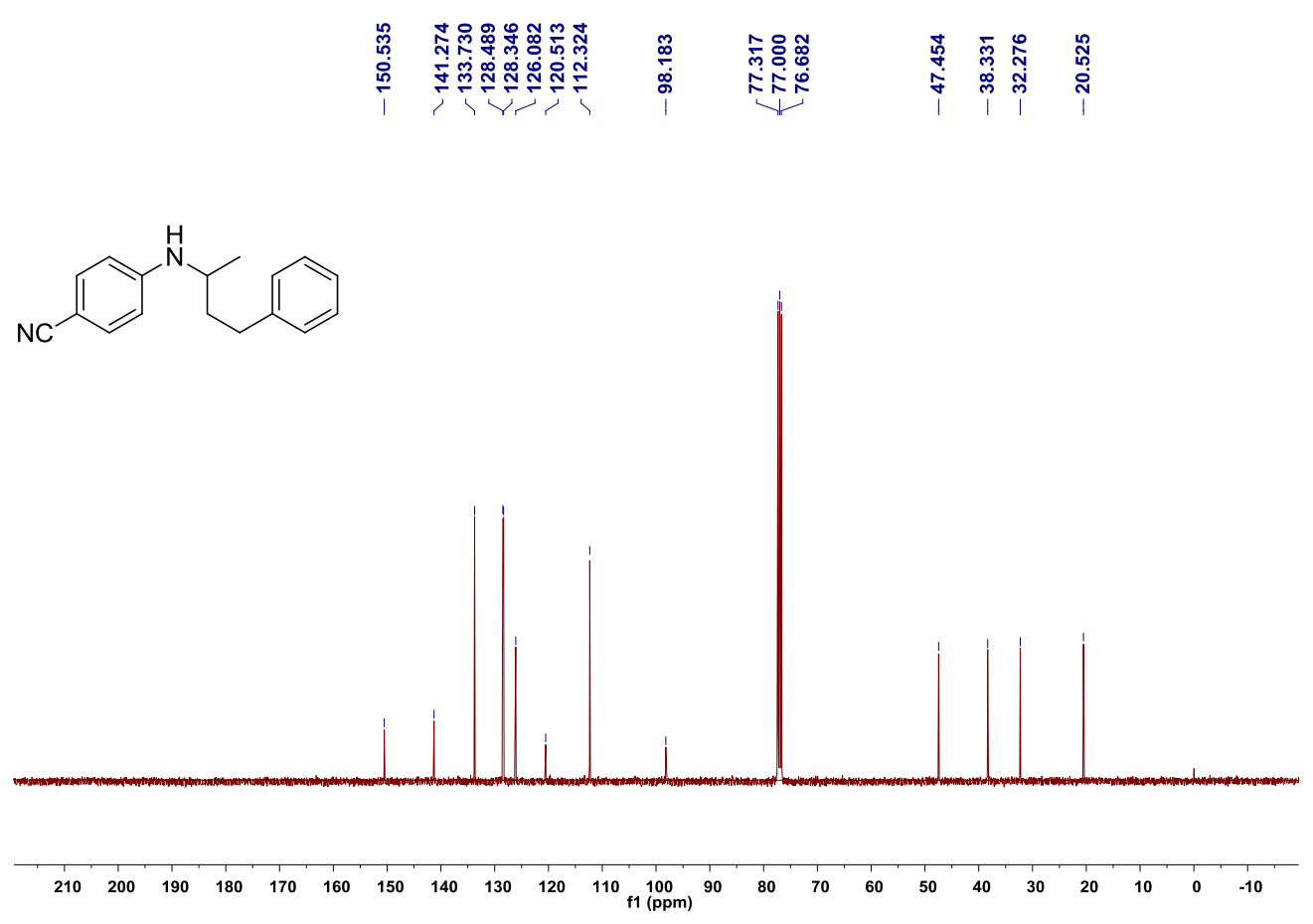

150.368
133.628
120.649
112.192
97.610
77.318
77.000
76.682
51.100
32.836
25.546
24.705
H
N
NC
f1 (ppm)

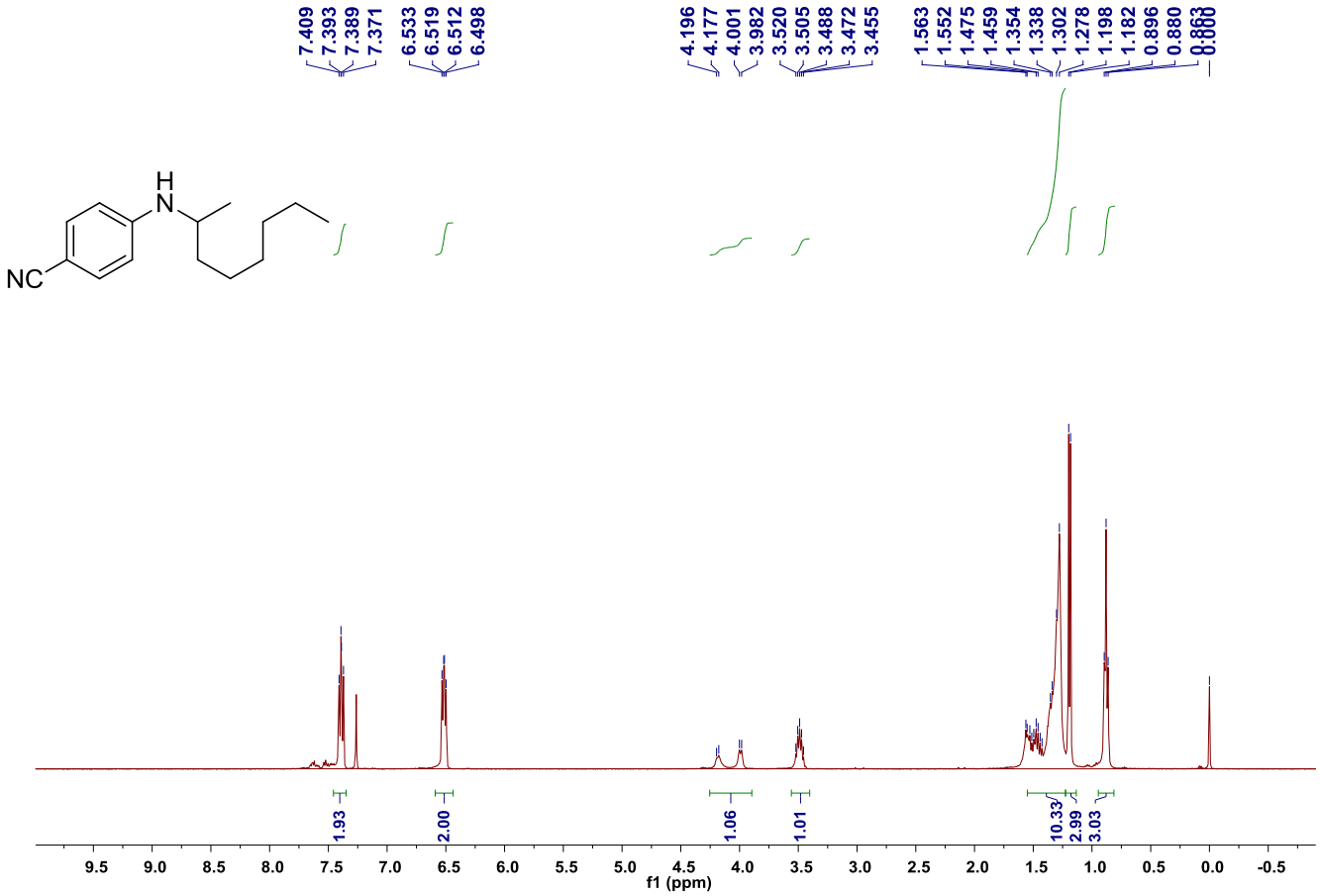

7.425
7.403
7.268
6.576
6.554
4.238
3.495
3.472
3.449
2.158
2.143
2.122
2.107
2.082
1.936
1.915
1.904
1.895
1.885
1.869
1.651
1.627
1.598
0.000
H
N
NC
F
F
1.97
2.00
0.98
1.00
4.06
2.08
2.07
f1 (ppm)

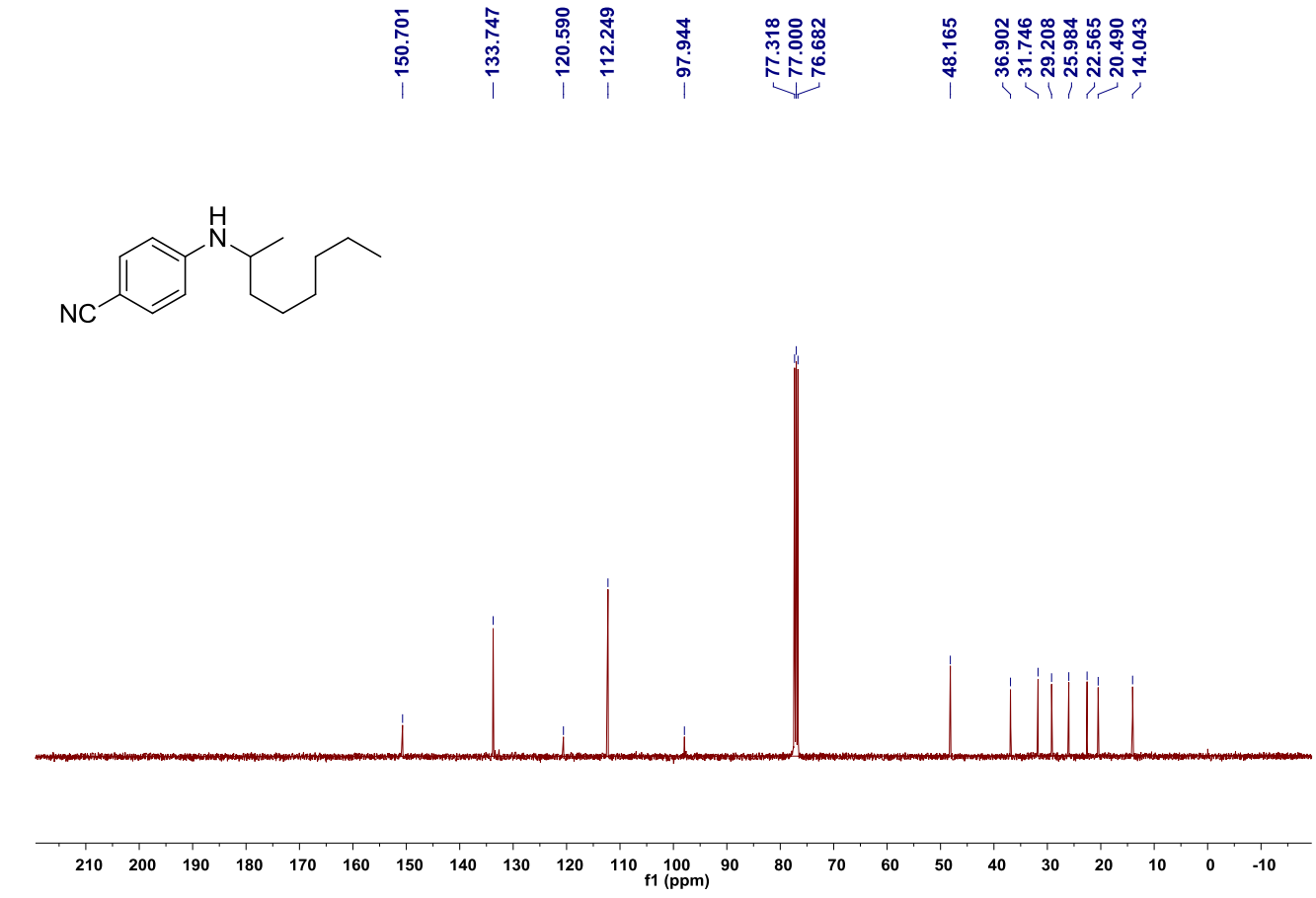

150.040
133.744
124.780
122.383
120.313
119.976
112.429
98.717
77.318
77.000
76.682
48.948
32.088
31.840
31.593
28.385
28.301
H
N
NC
F
F
f1 (ppm)


-95.222
-95.854
-99.838
-100.476
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


7.387
7.365
7.306
7.289
7.270
7.225
7.206
7.188
7.164
7.147
6.448
6.426
4.013
3.994
3.526
3.510
3.490
2.725
2.709
2.690
1.871
1.851
1.230
-0.000
NC
H
N
2.01
2.05
2.98
2.00
1.01
1.06
2.07
2.11
3.13
f1 (ppm)


150.535
141.274
133.730
128.489
128.346
126.082
120.513
112.324
98.183
77.317
77.000
76.682
47.454
38.331
32.276
20.525
NC
H
N
f1 (ppm)


7.409
7.393
7.389
7.371
6.533
6.519
6.512
6.498
4.196
4.177
4.001
3.982
3.520
3.505
3.488
3.472
3.455
1.563
1.552
1.475
1.459
1.354
1.338
1.302
1.278
1.198
1.182
0.896
0.880
H
N
NC
1.93
2.00
1.06
1.01
10.33
2.99
3.03
f1 (ppm)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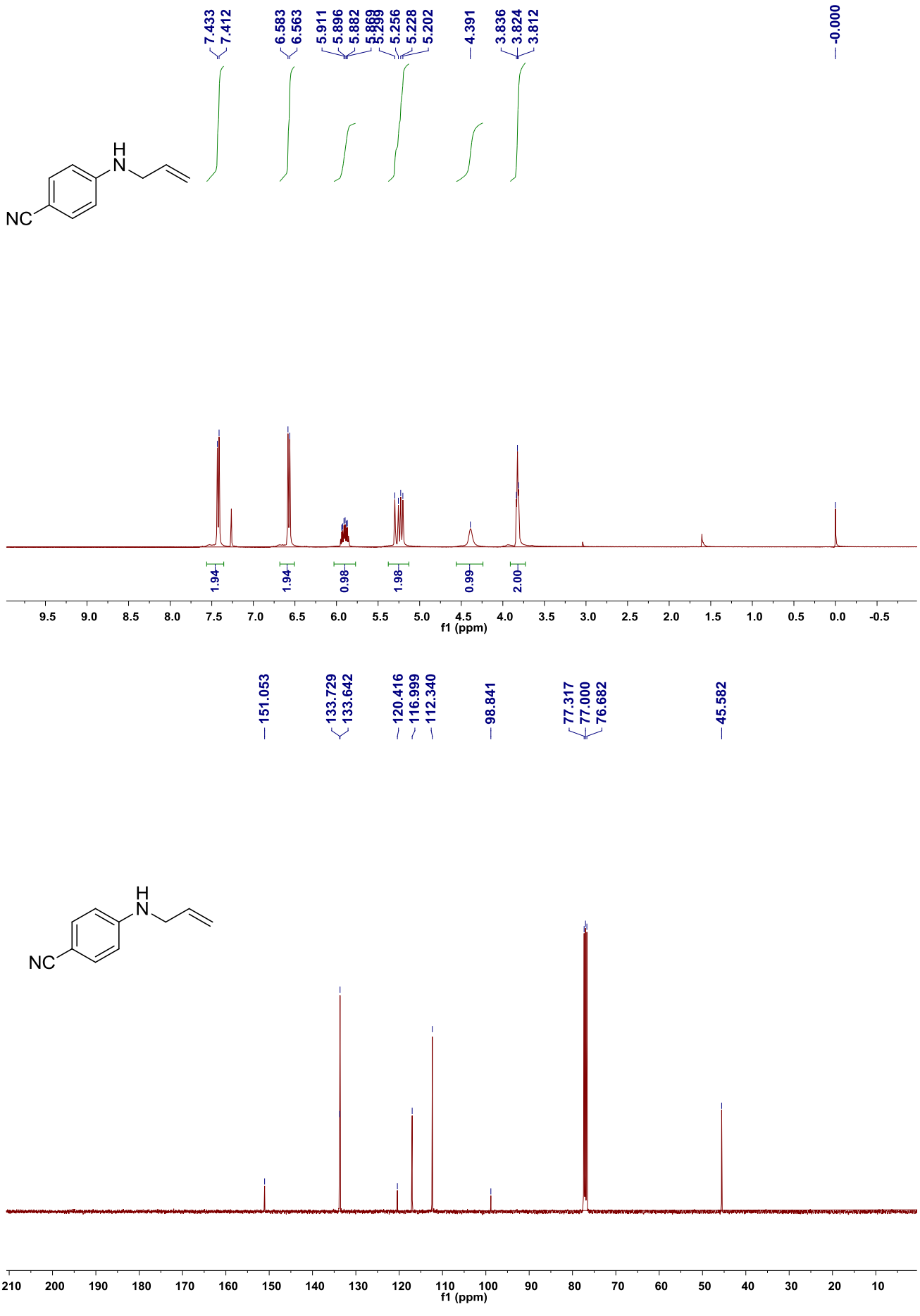
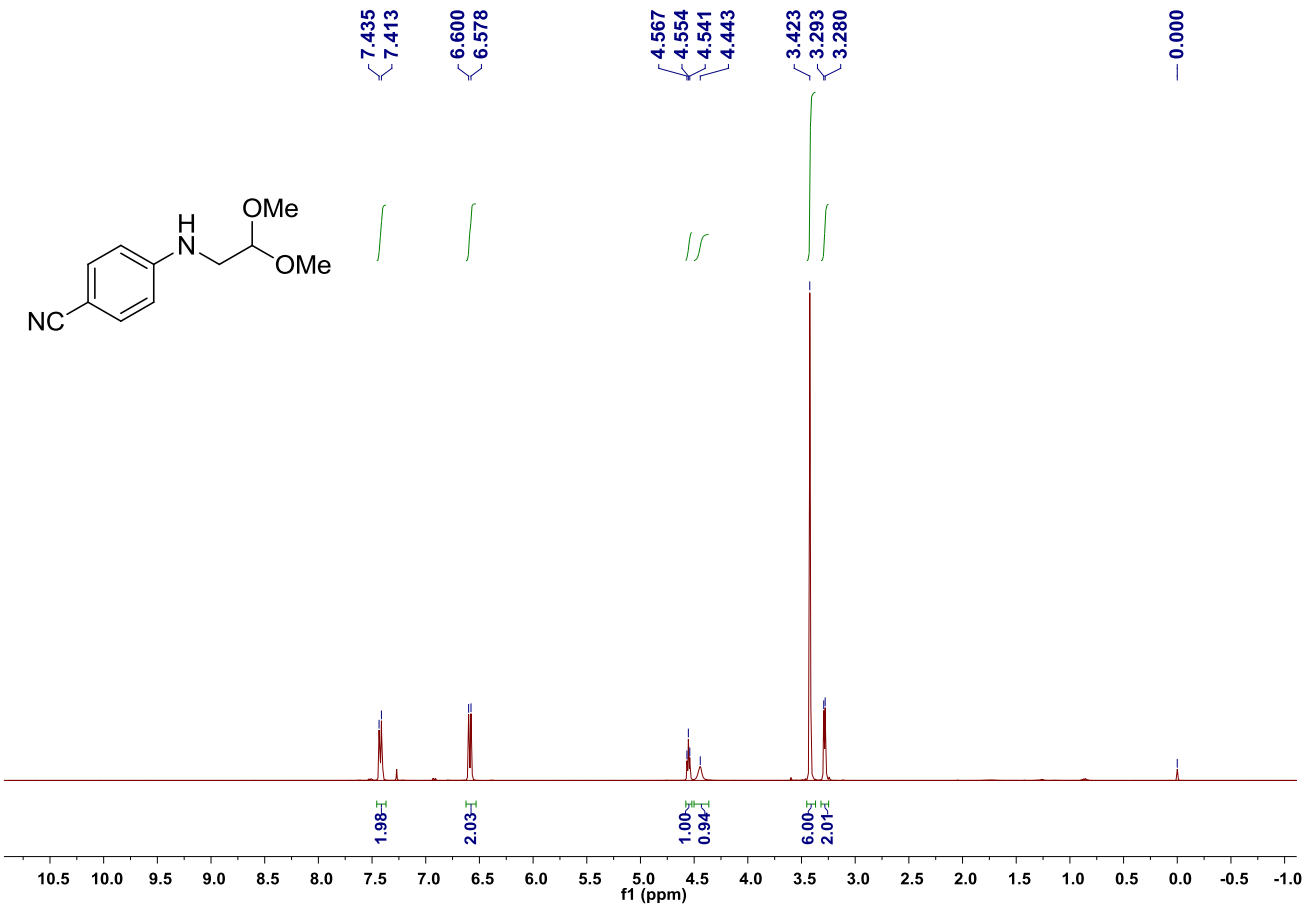
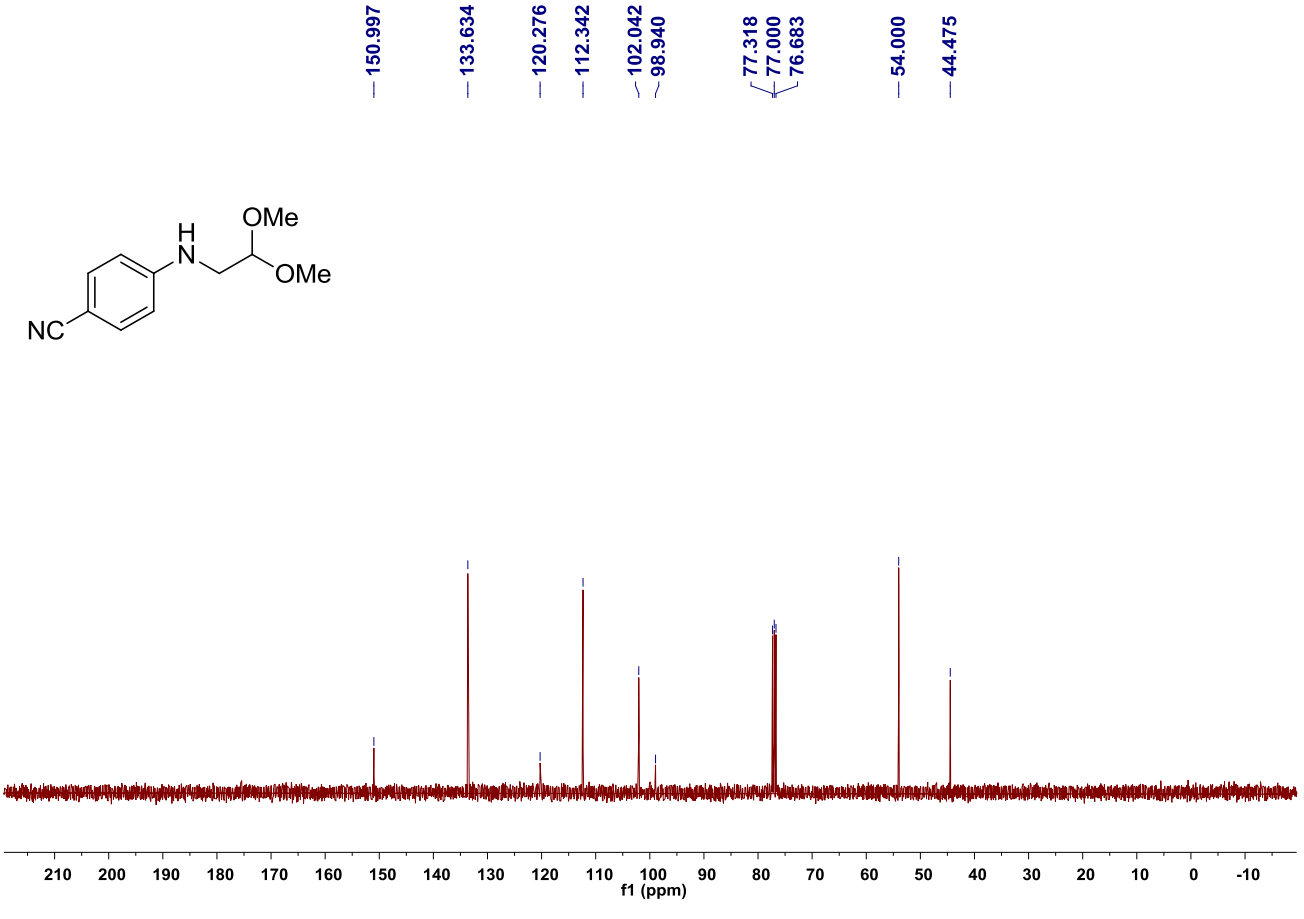
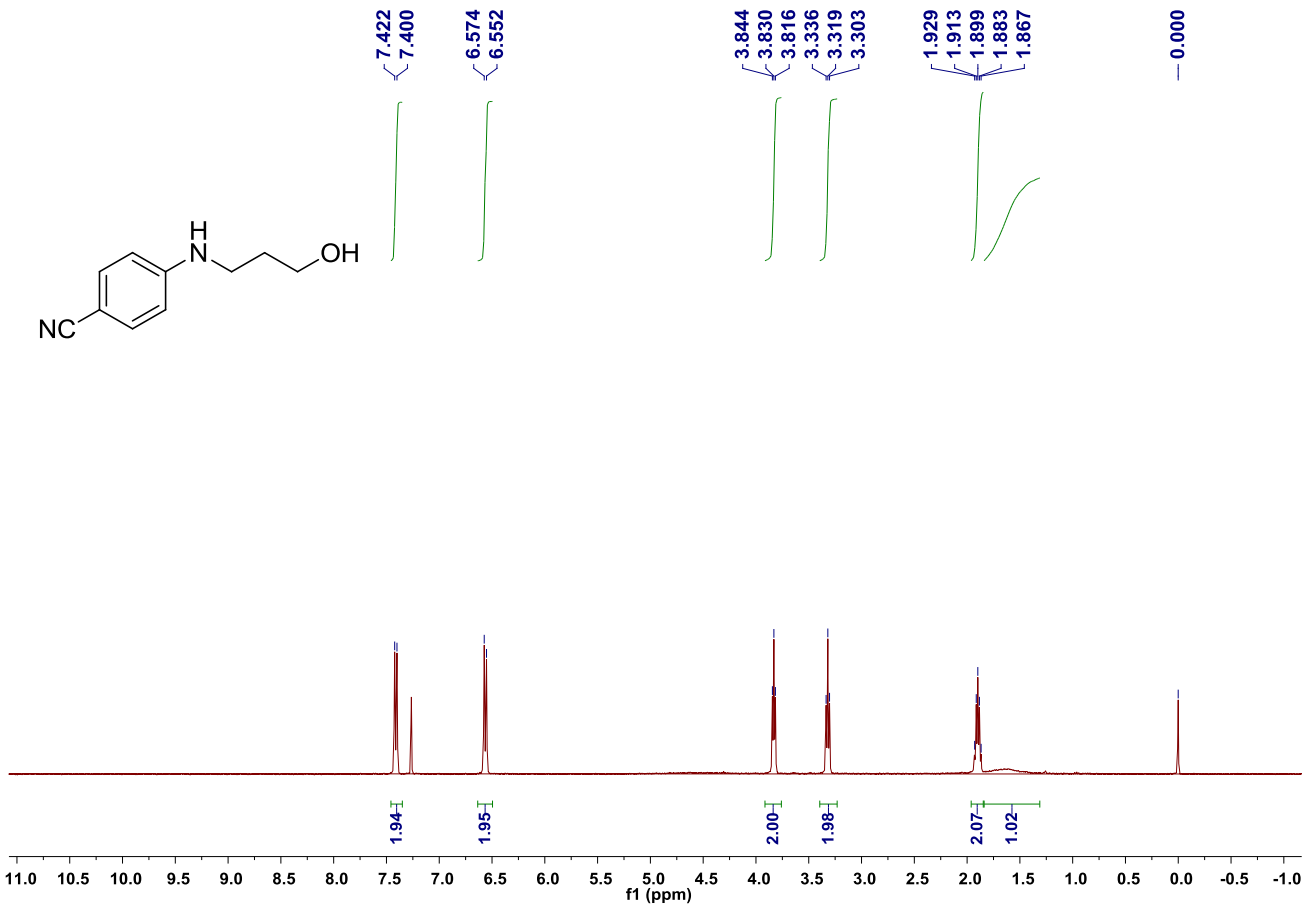
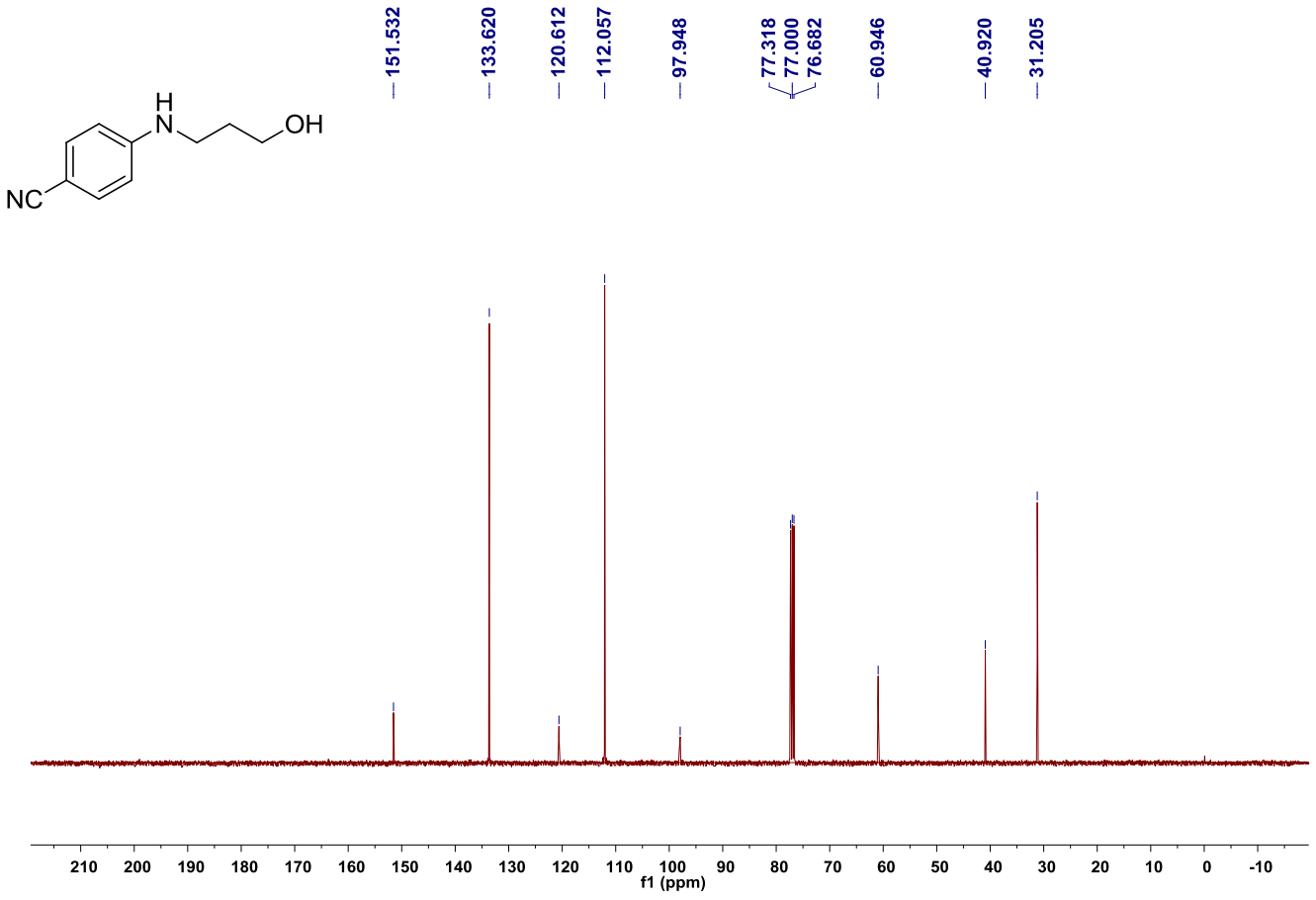
133.747
120.590
112.249
97.944
77.318
77.000
76.682
48.165
36.902
31.746
29.208
25.984
22.565
20.490
14.043
H
N
NC
f1 (ppm)

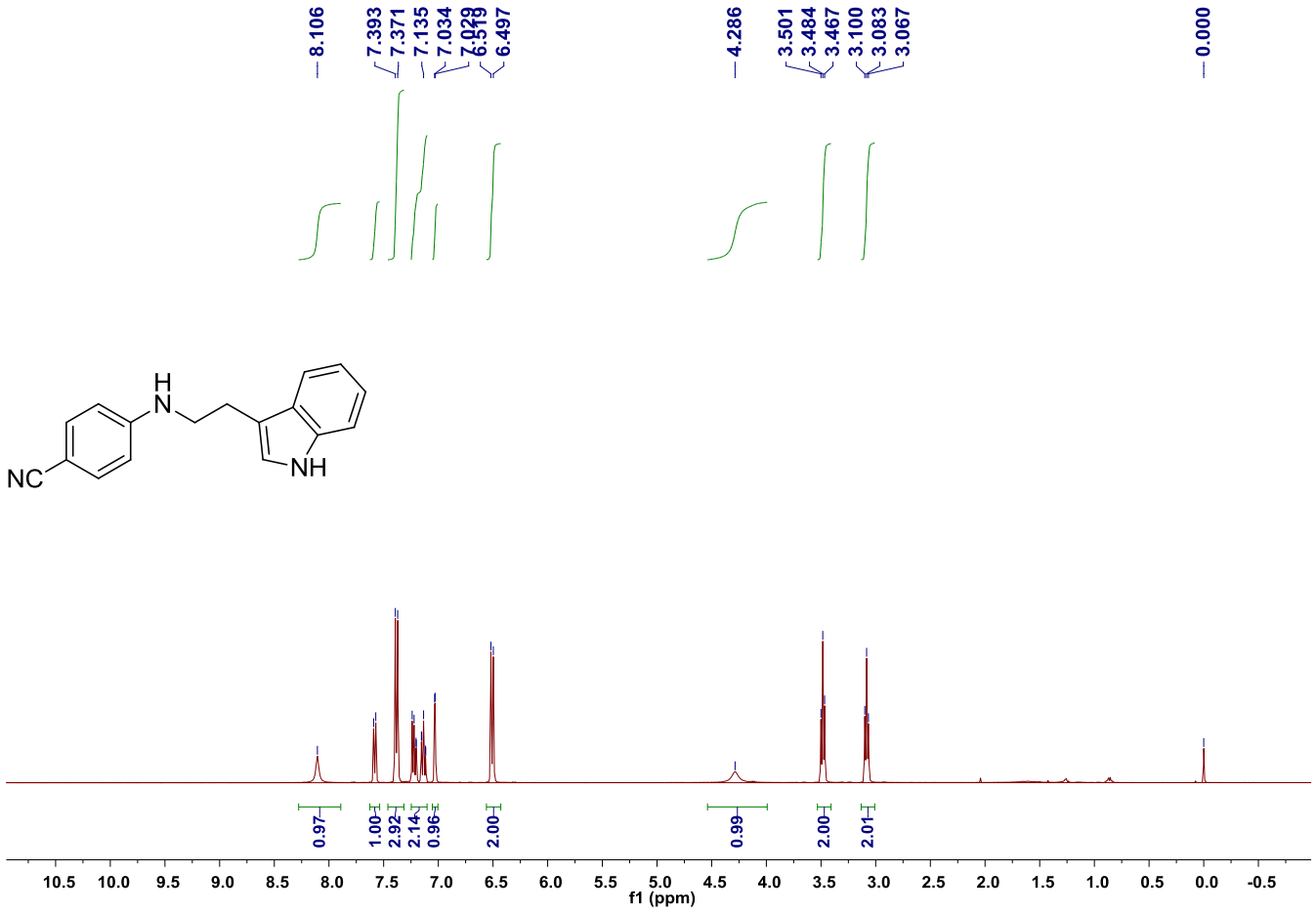

7.433
7.412
6.583
6.563
5.911
5.896
5.882
5.256
5.228
5.202
4.391
3.836
3.824
3.812
-0.000
H
N
NC
1.94
1.94
0.98
1.98
0.99
2.00
f1 (ppm)
151.053
133.729
133.642
120.416
116.999
112.340
98.841
77.317
77.000
76.682
45.582
H
N
NC
f1 (ppm)

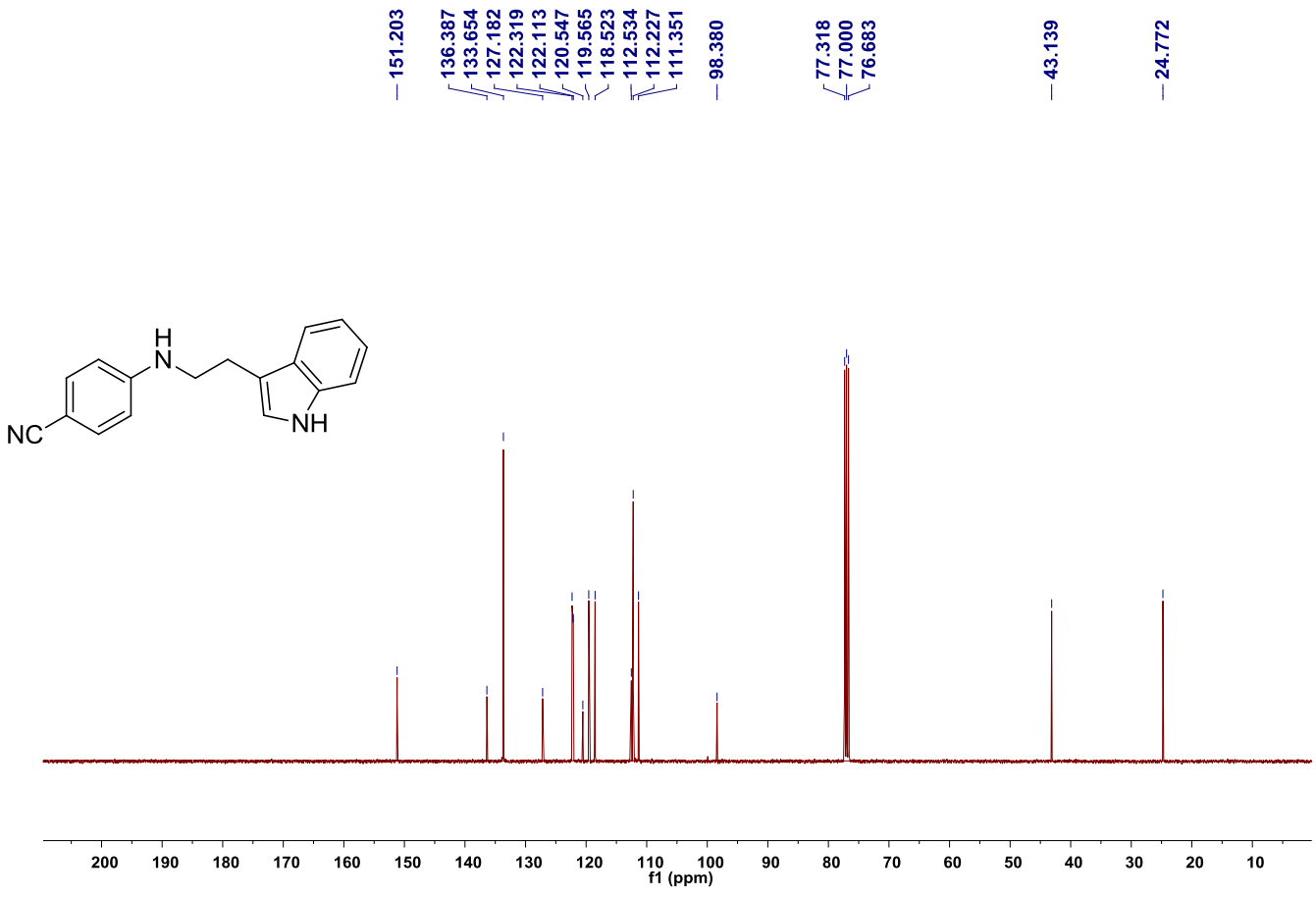

7.435
7.413
6.600
6.578
4.567
4.554
4.541
4.443
3.423
3.293
3.280
0.000
OMe
H
N
OMe
NC
1.98
2.03
1.00
0.94
6.00
2.01
f1 (ppm)

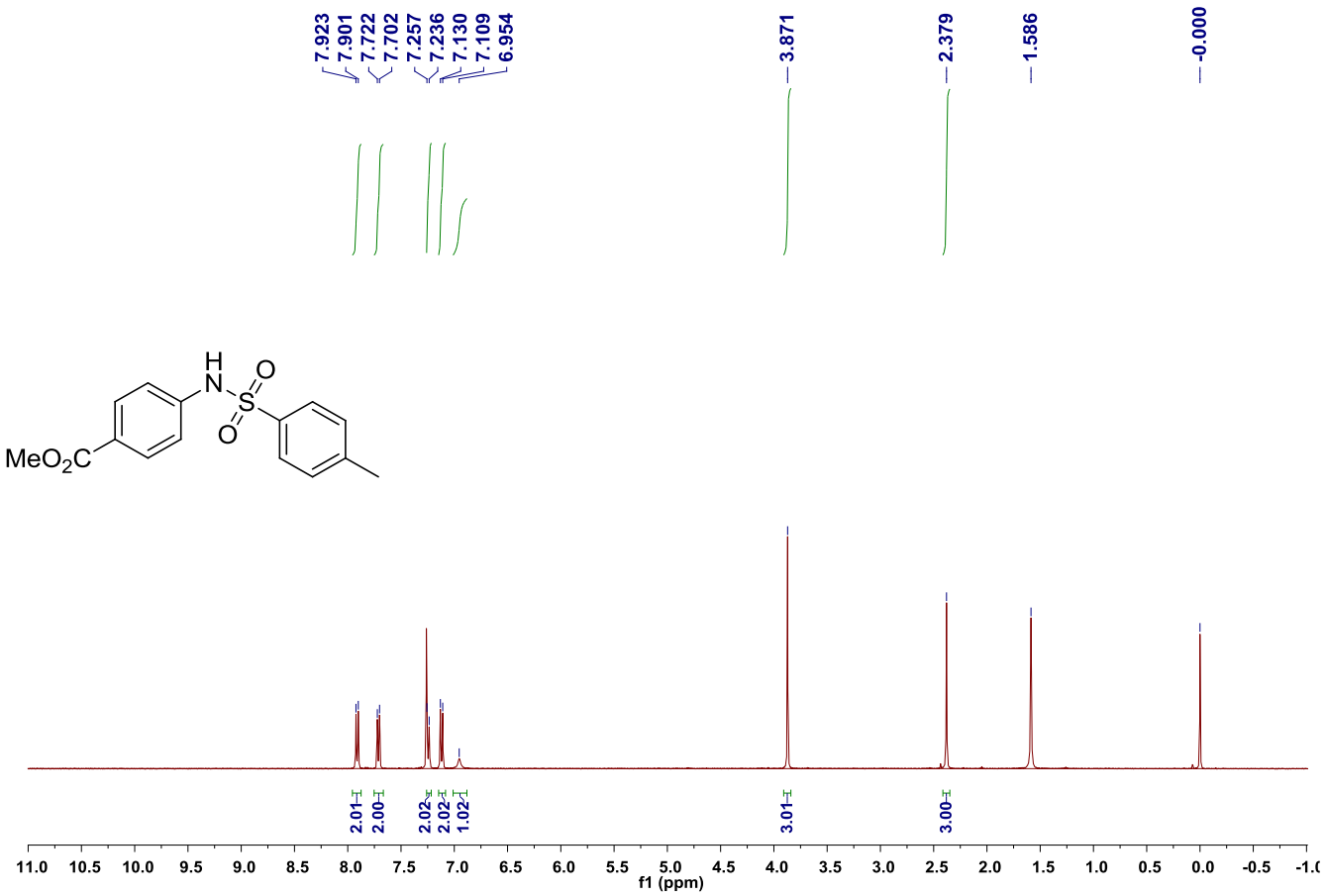

150.997
133.634
120.276
112.342
102.042
98.940
77.318
77.000
76.683
54.000
44.475
OMe
H
N
OMe
NC
f1 (ppm)

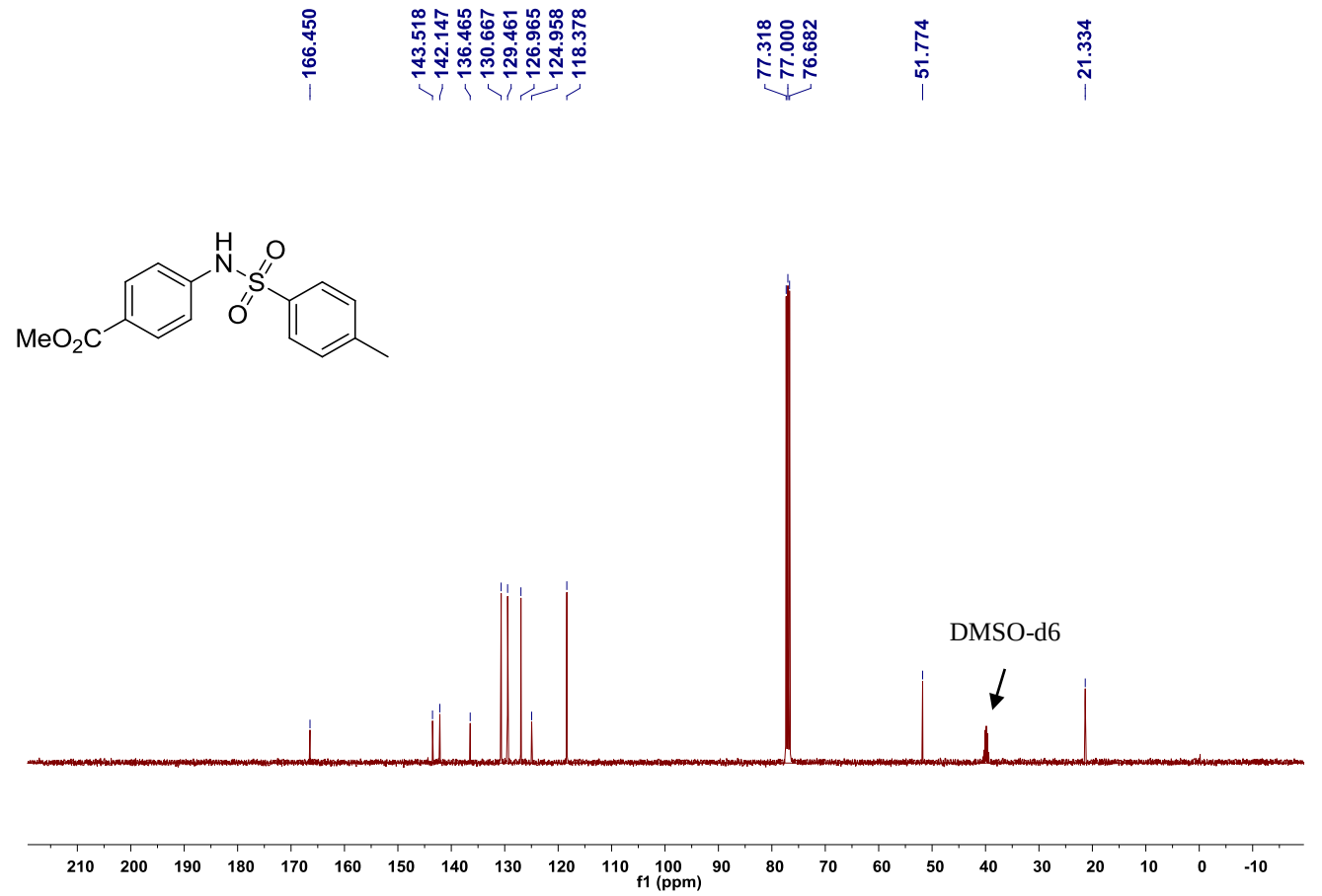

7.422
7.400
6.574
6.552
3.844
3.830
3.816
3.336
3.319
3.303
1.929
1.913
1.899
1.883
1.867
0.000
H
N
OH
NC
1.94
1.95
2.00
1.98
2.07
1.02
f1 (ppm)

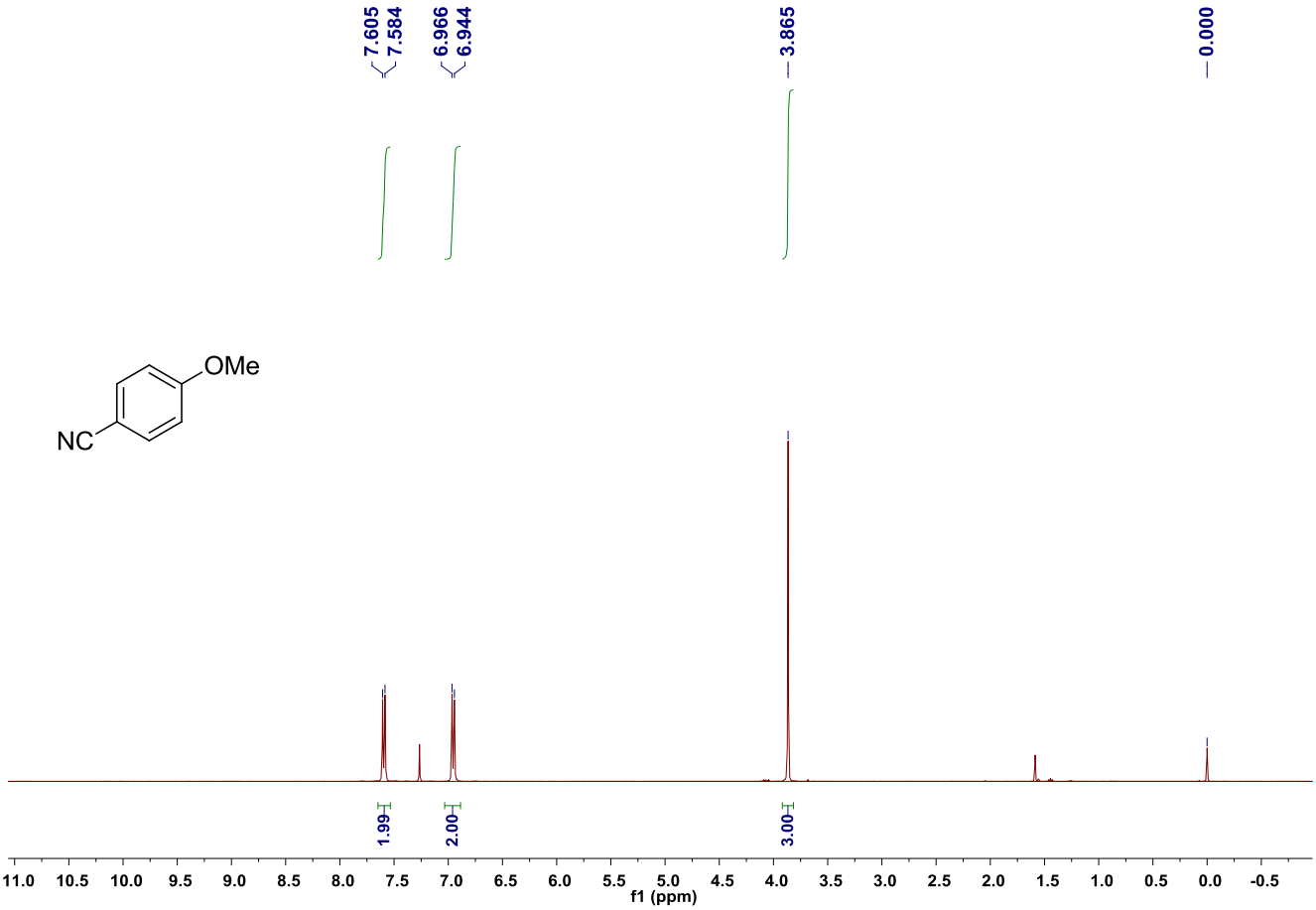

151.532
133.620
120.612
112.057
97.948
77.318
77.000
76.682
60.946
40.920
31.205
H
N
OH
NC
f1 (ppm)

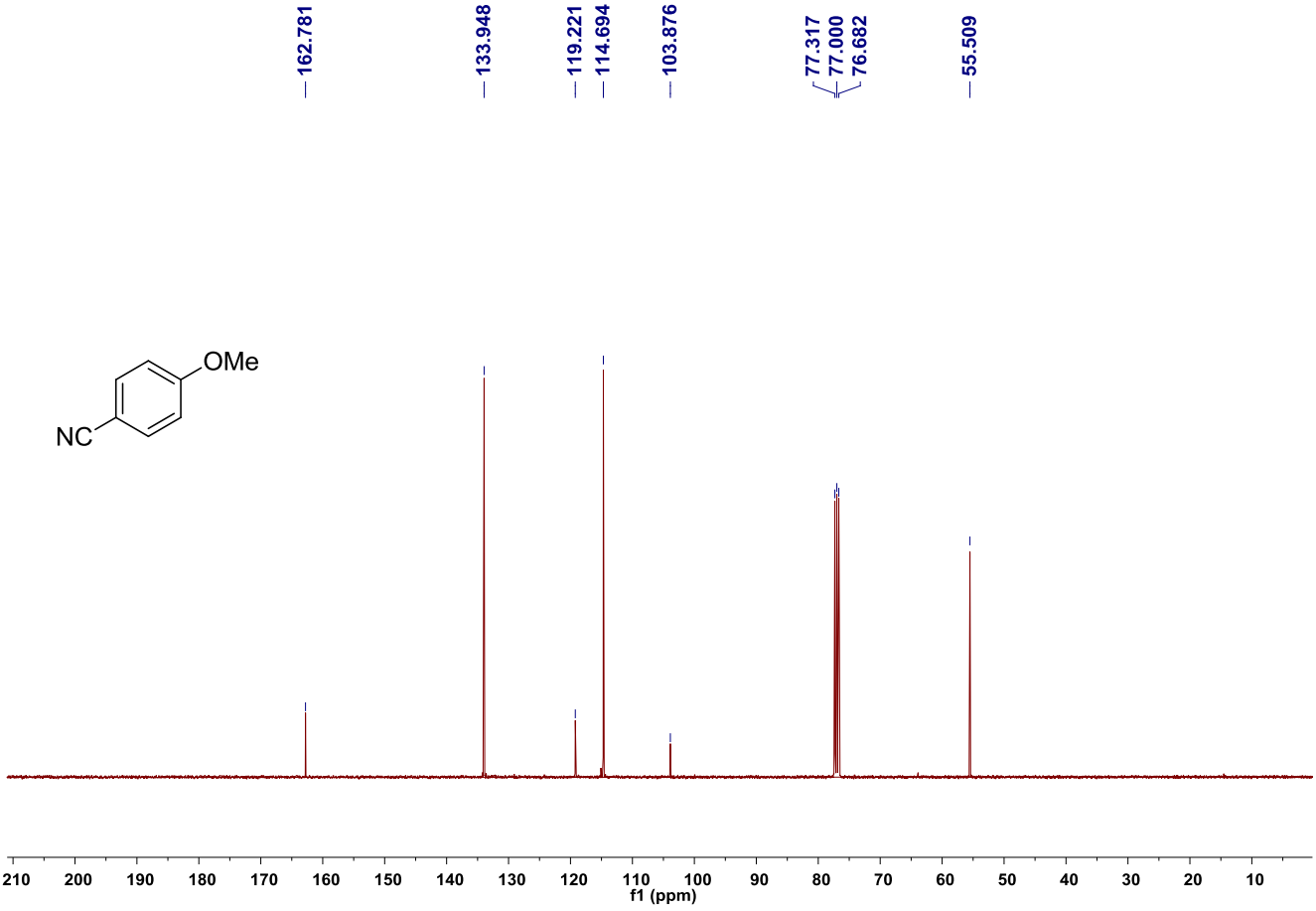

8.106
7.393
7.371
7.135
7.034
7.029
6.519
6.497
4.286
3.501
3.484
3.467
3.100
3.083
3.067
0.000
NC
H
N
NH
0.97
1.00
2.92
2.14
0.96
2.00
0.99
2.00
2.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

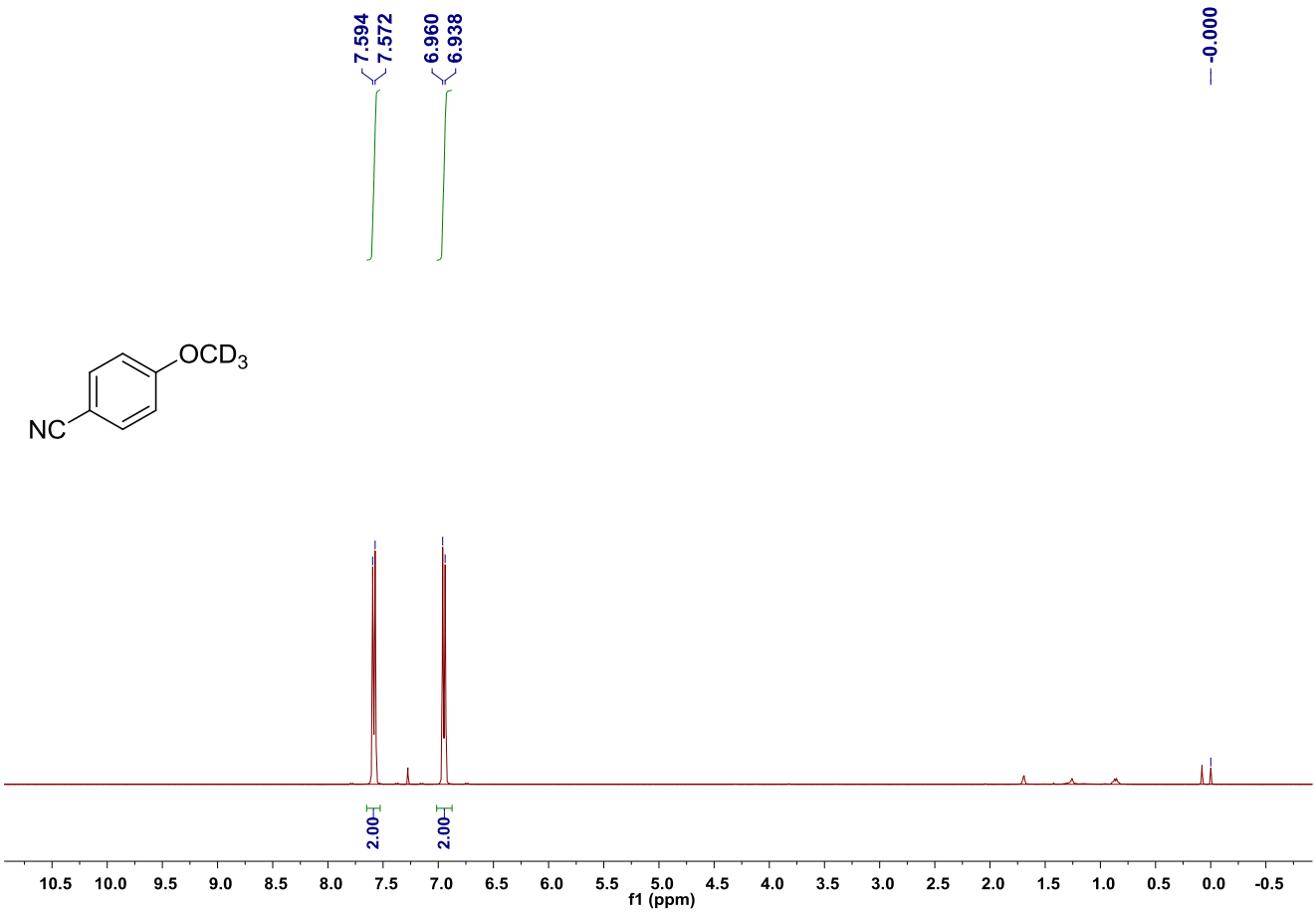

151.203
136.387
133.654
127.182
122.319
122.113
120.547
119.565
118.523
112.534
112.227
111.351
98.380
77.318
77.000
76.683
43.139
24.772
NC
H
N
NH
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

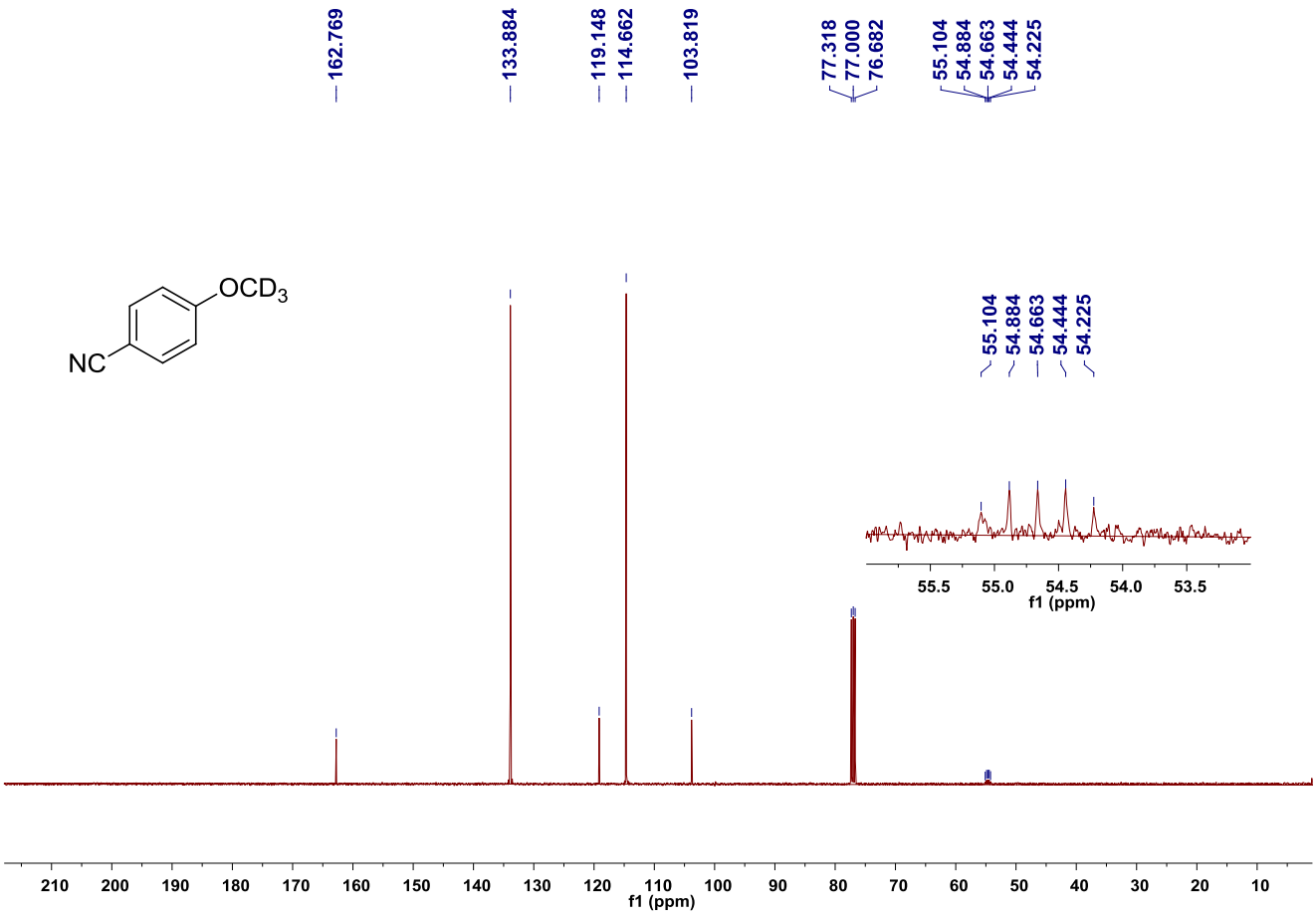

7.923
7.901
7.722
7.702
7.257
7.236
7.130
7.109
6.954
3.871
2.379
1.586
-0.000
MeO2C
2.01
2.00
2.02
2.02
1.02
3.01
3.00
f1 (ppm)

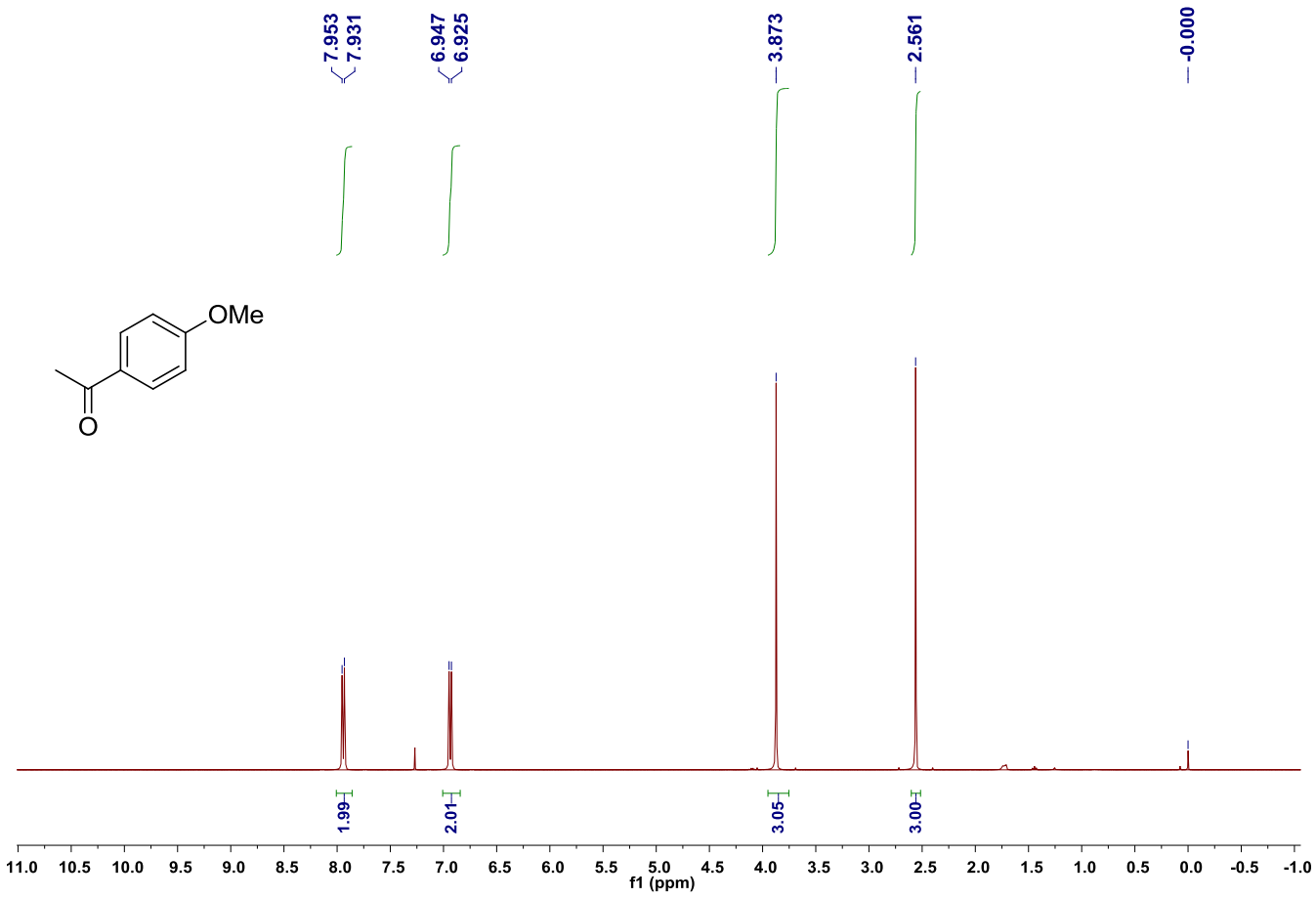

166.450
143.518
142.147
136.465
130.667
129.461
126.965
124.958
118.378
77.318
77.000
76.682
51.774
21.334
MeO2C
DMSO-d6
f1 (ppm)

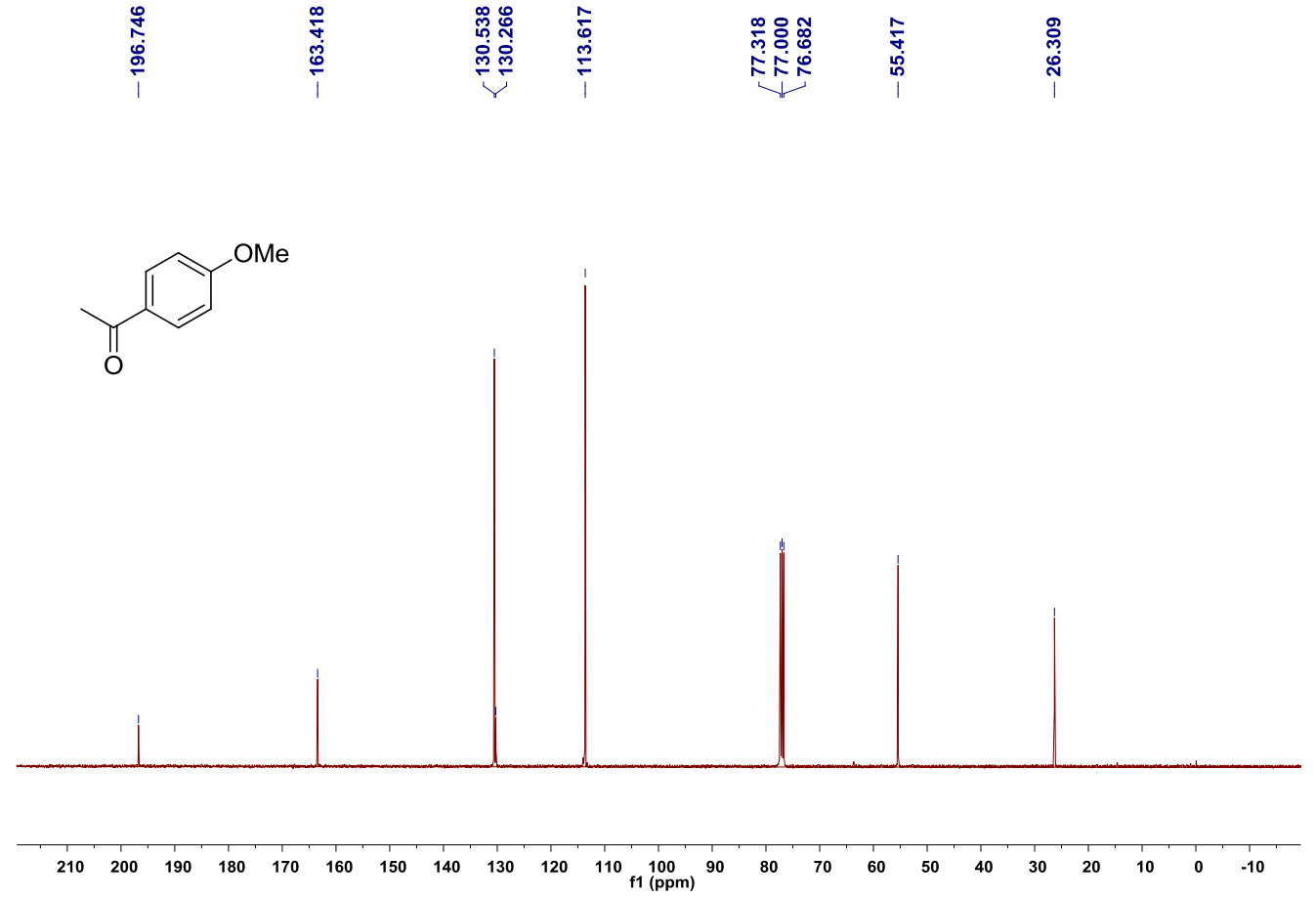

7.605
7.584
6.966
6.944
3.865
0.000
OMe
NC
1.99
2.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

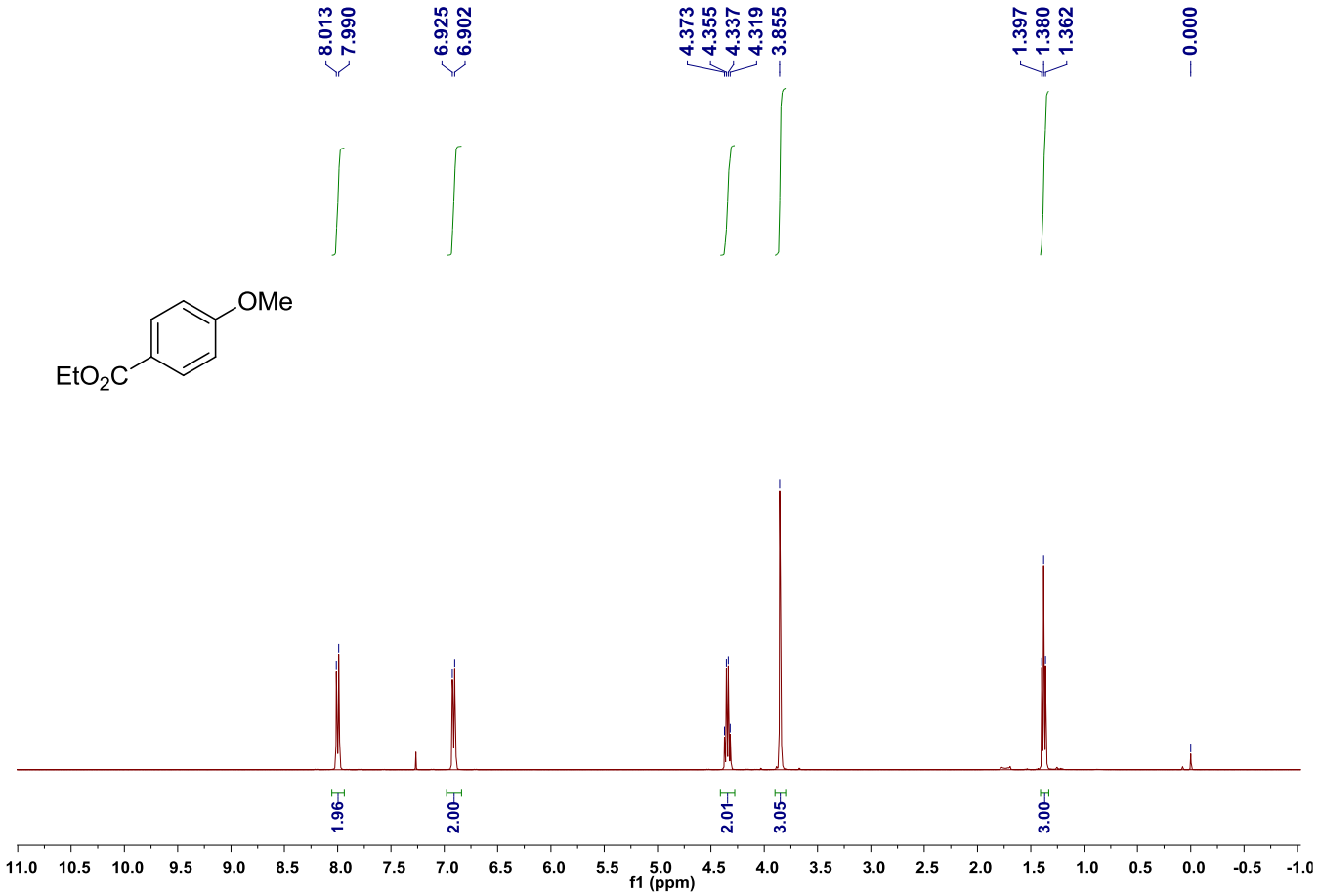

162.781
133.948
119.221
114.694
103.876
77.317
77.000
76.682
55.509
OMe
NC
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

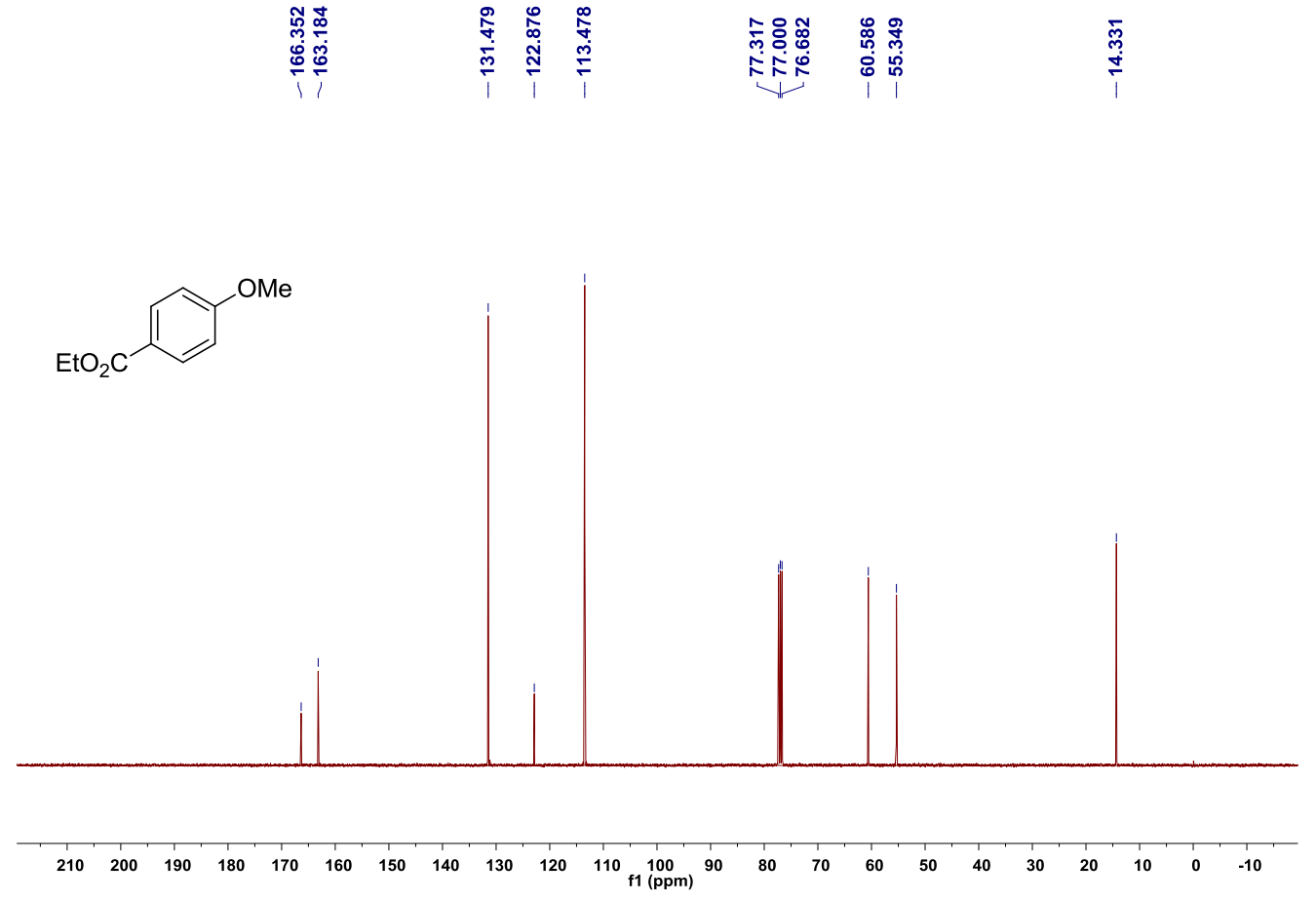

7.594
7.572
6.960
6.938
-0.000
OCD3
NC
2.00
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


162.769
133.884
119.148
114.662
103.819
77.318
77.000
76.682
55.104
54.884
54.663
54.444
54.225
OCD3
NC
55.5 55.0 54.5 54.0 53.5
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.953
7.931
6.947
6.925
3.873
2.561
-0.000
OMe
O
1.99
2.01
3.05
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


196.746
163.418
130.538
130.266
113.617
77.318
77.000
76.682
55.417
26.309
OMe
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.013
7.990
6.925
6.902
4.373
4.355
4.337
4.319
3.855
1.397
1.380
1.362
0.000
OMe
EtO2C
1.96
2.00
2.01
3.05
3.00
f1 (ppm)


166.352
163.184
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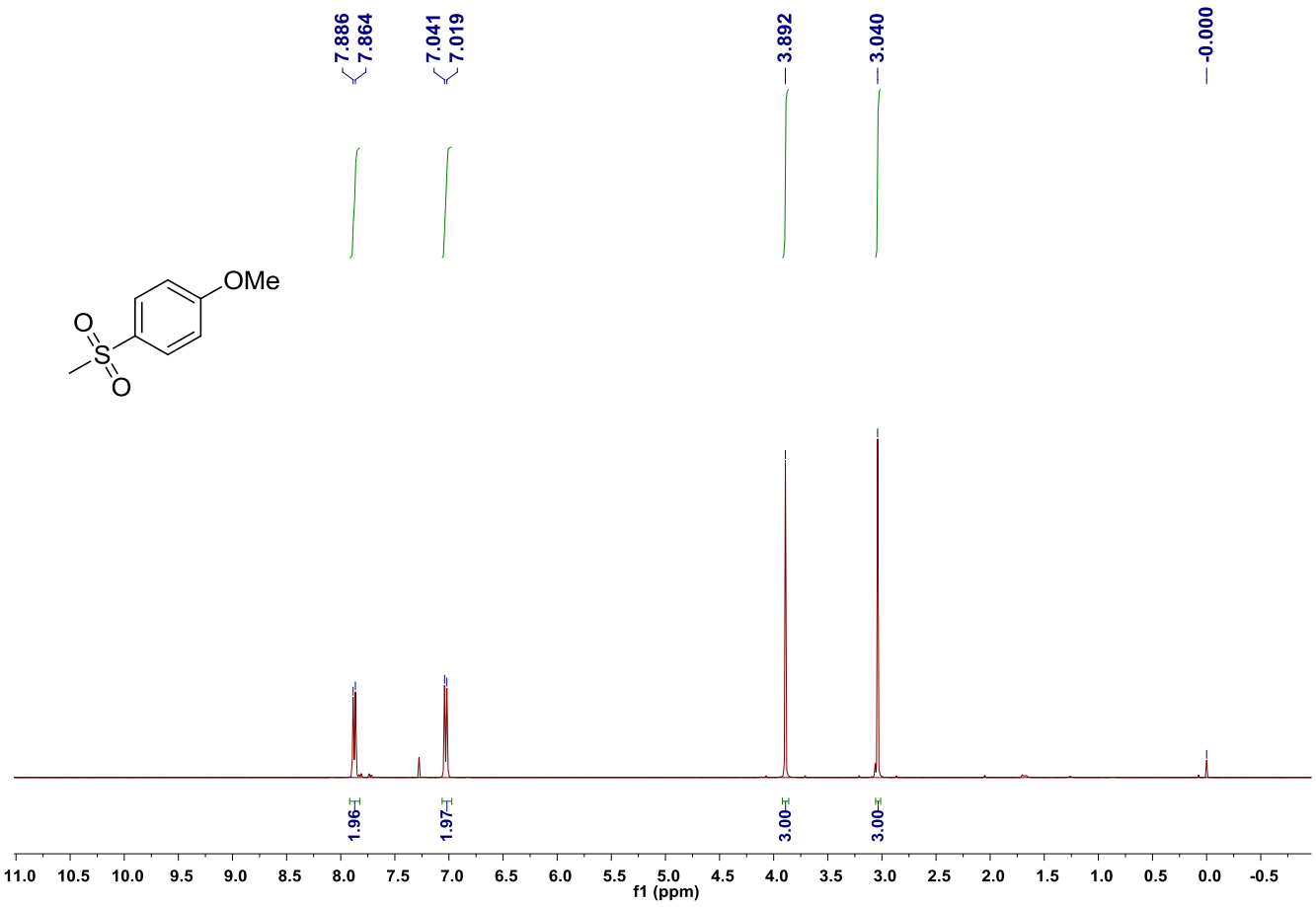
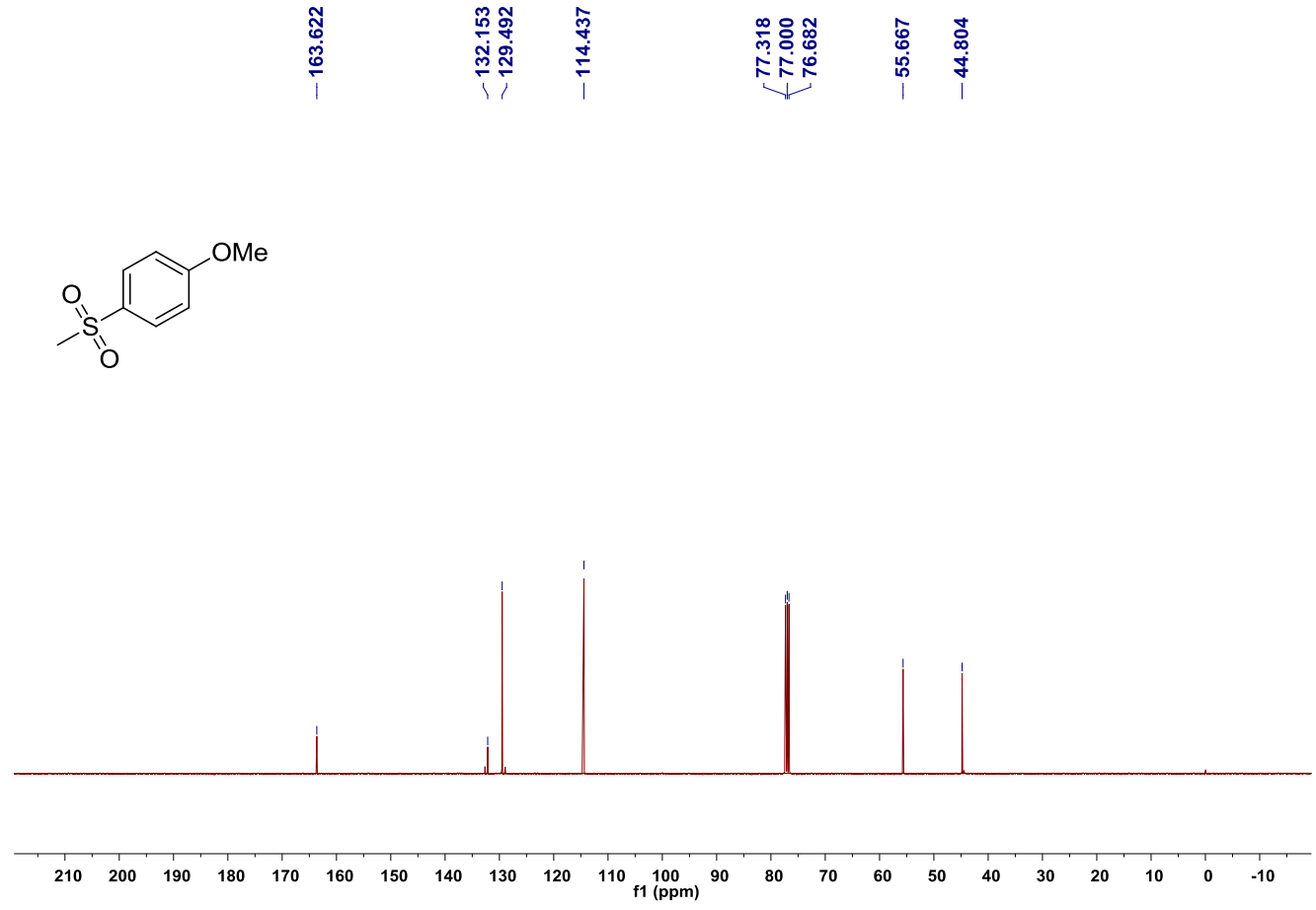
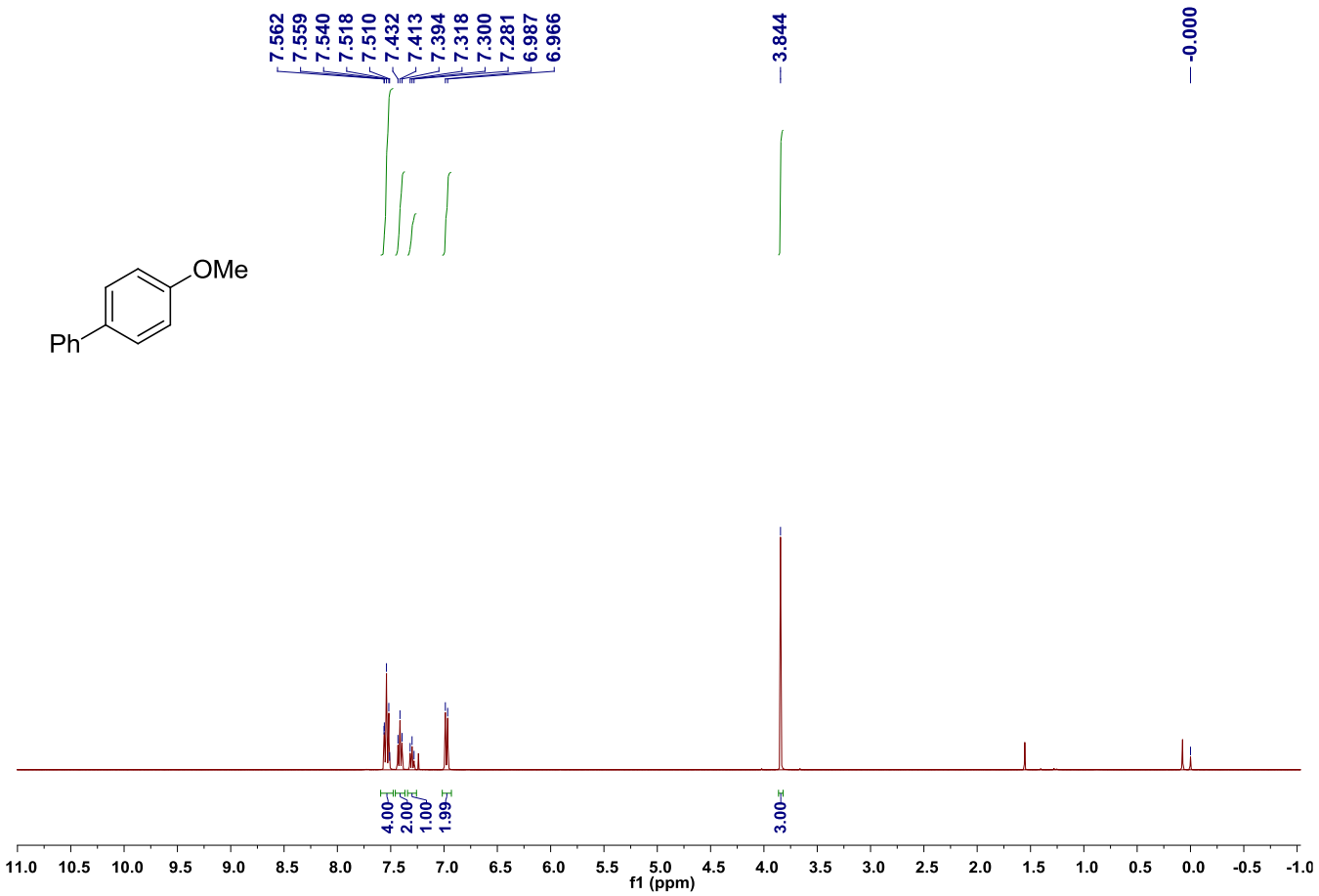
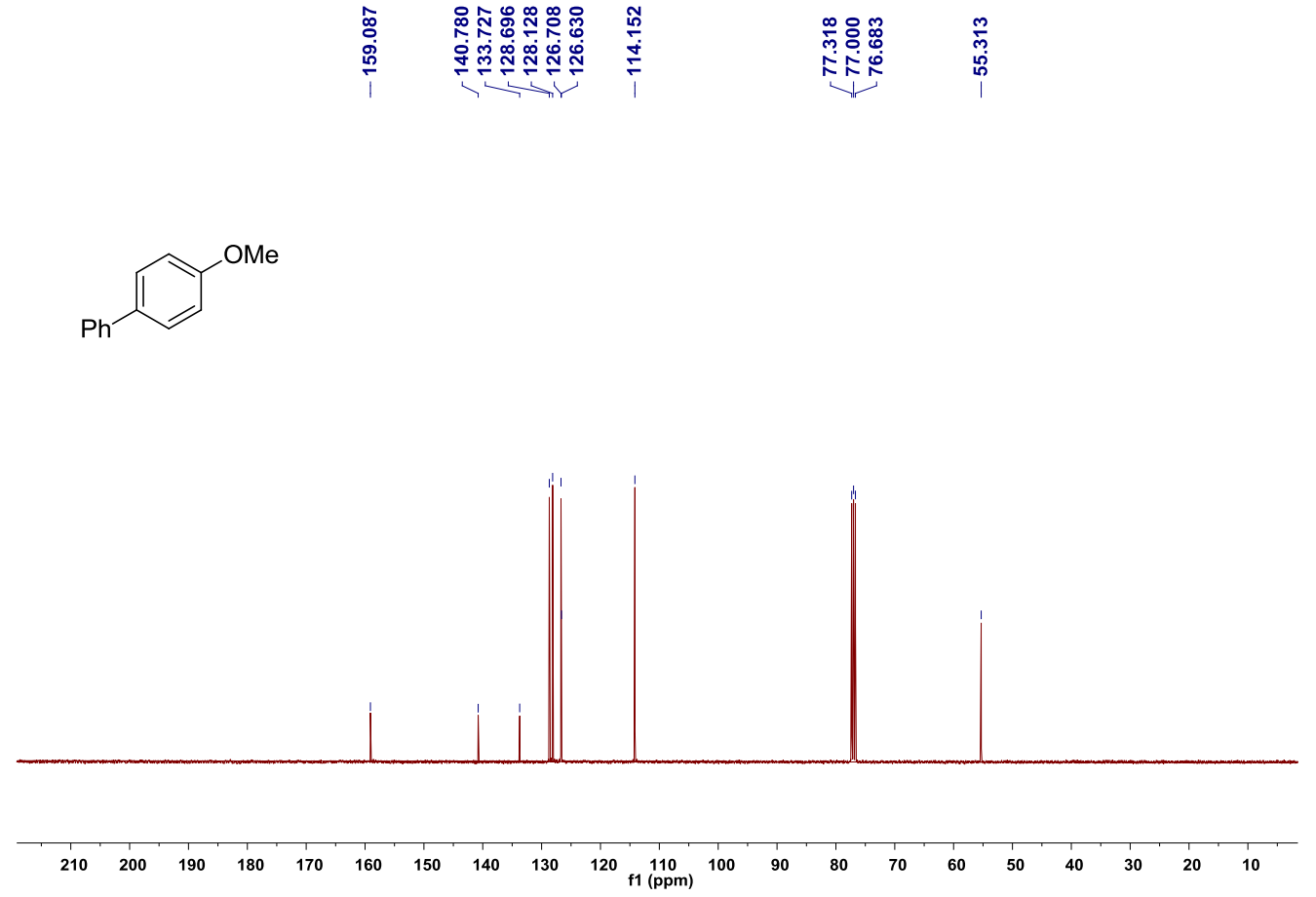
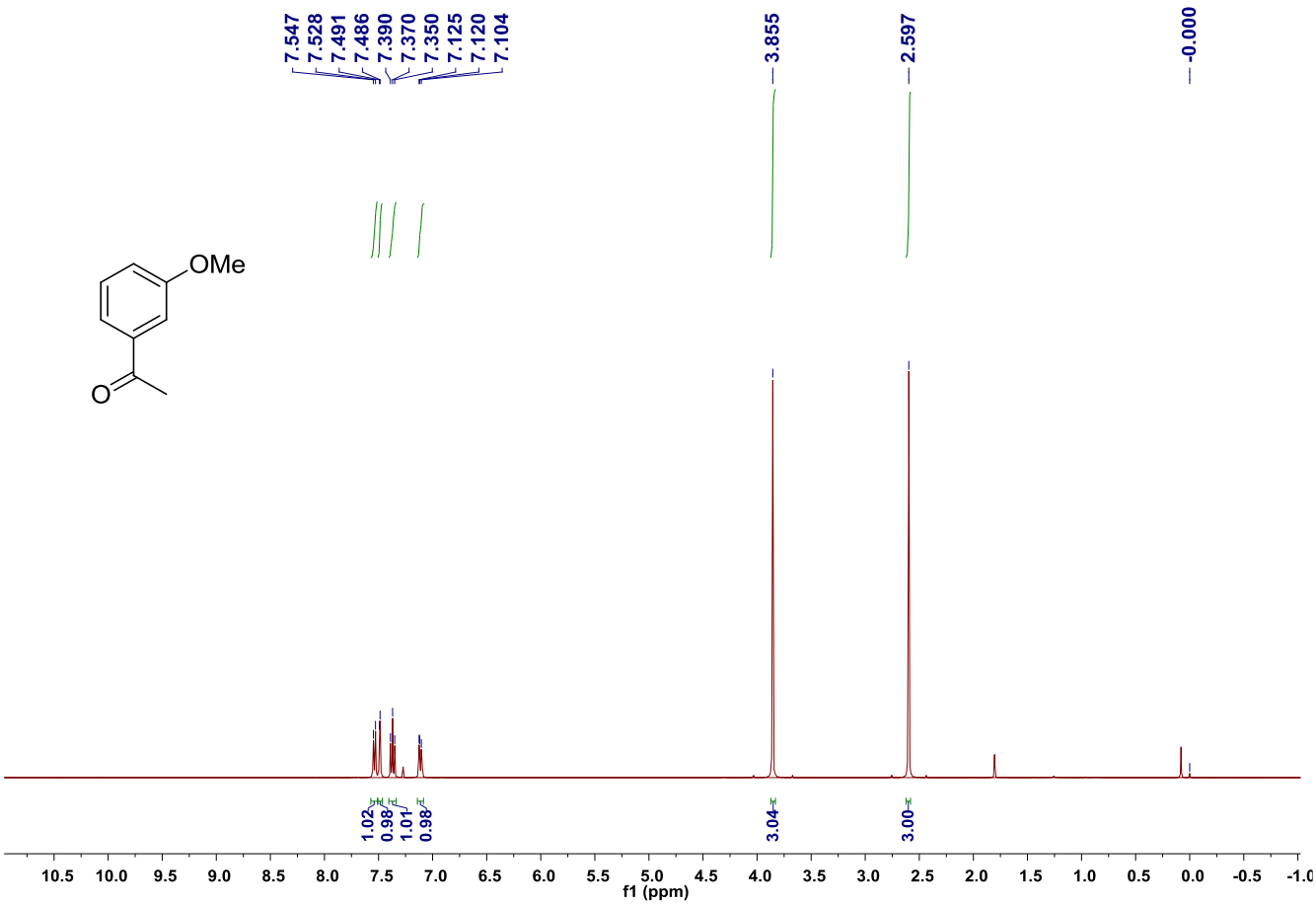
122.876
113.478
77.317
77.000
76.682
60.586
55.349
14.331
OMe
EtO2C
f1 (ppm)

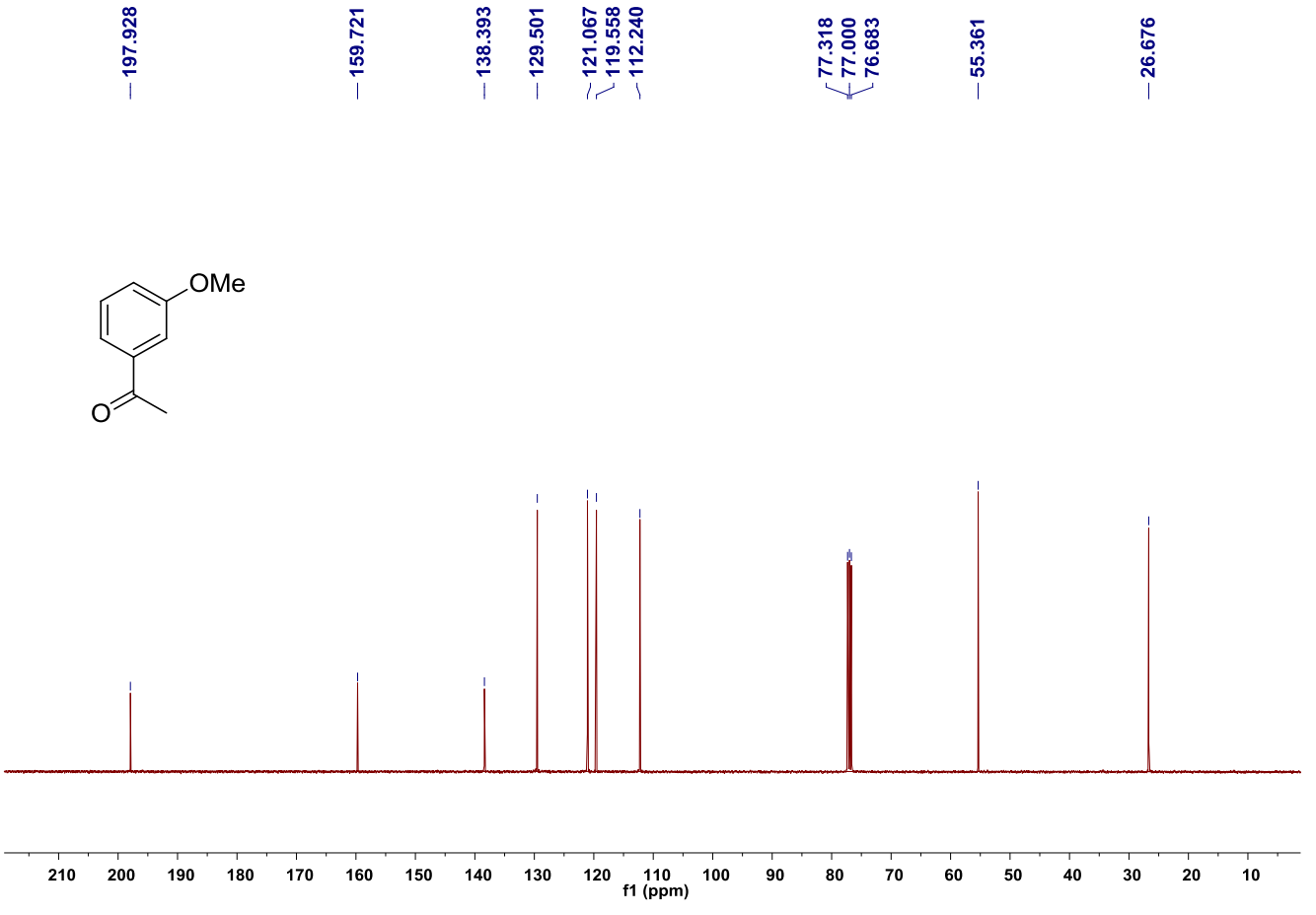

7.886
7.864
7.041
7.019
3.892
3.040
-0.000
OMe
O
S
O
1.96
1.97
3.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


163.622
132.153
129.492
114.437
77.318
77.000
76.682
55.667
44.804
OMe
O
S
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.562
7.559
7.540
7.518
7.510
7.432
7.413
7.394
7.318
7.300
7.281
6.987
6.966
3.844
-0.000
OMe
Ph
4.00
2.00
1.00
1.99
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


159.087
140.780
133.727
128.696
128.128
126.708
126.630
114.152
77.318
77.000
76.683
55.313
OMe
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.547
7.528
7.491
7.486
7.390
7.370
7.350
7.125
7.120
7.104
3.855
2.597
-0.000
OMe
O
1.02
0.98
1.01
0.98
3.04
3.00
f1 (ppm)


197.928
159.721
138.393
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119.558
112.240
77.318
77.000
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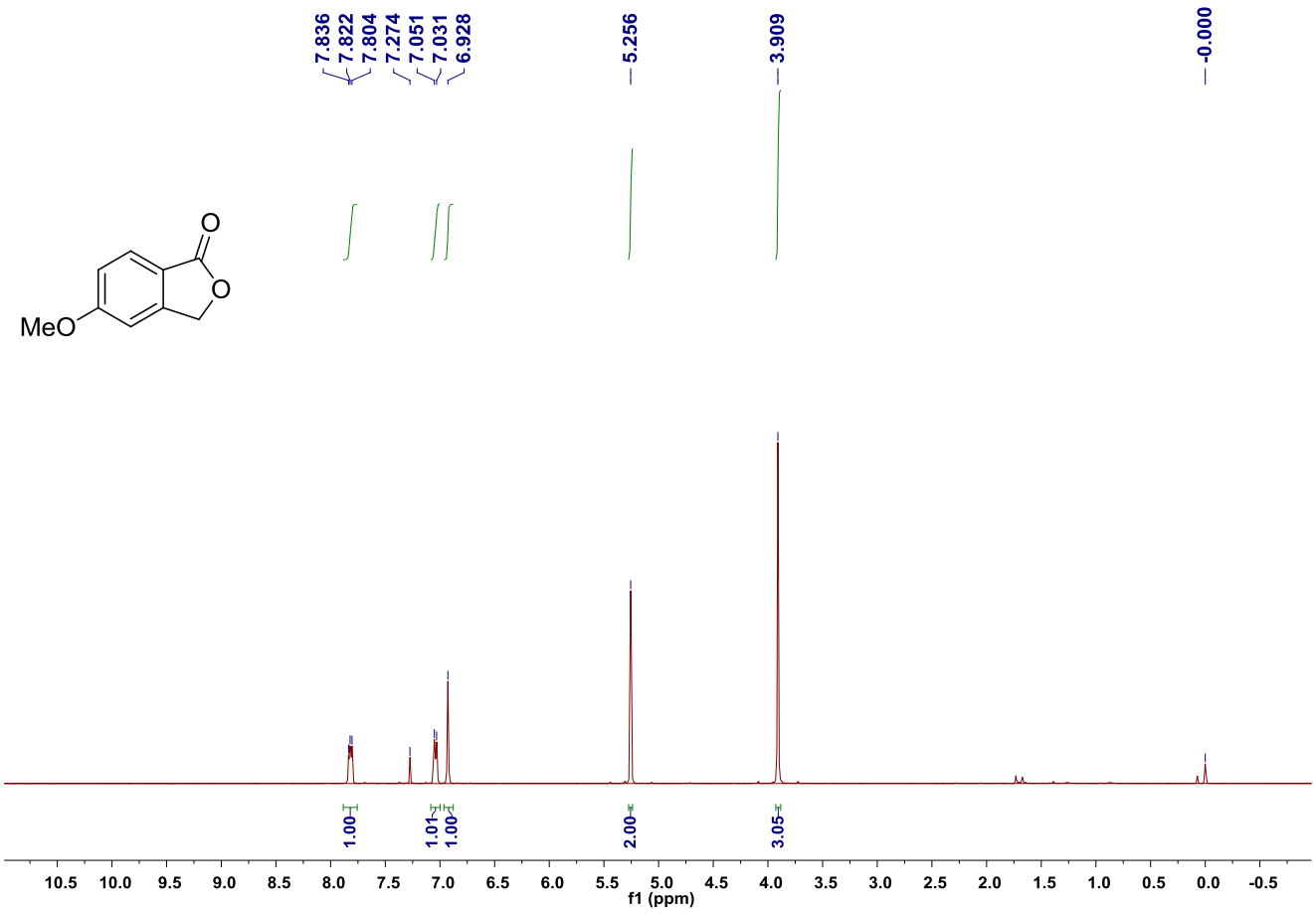
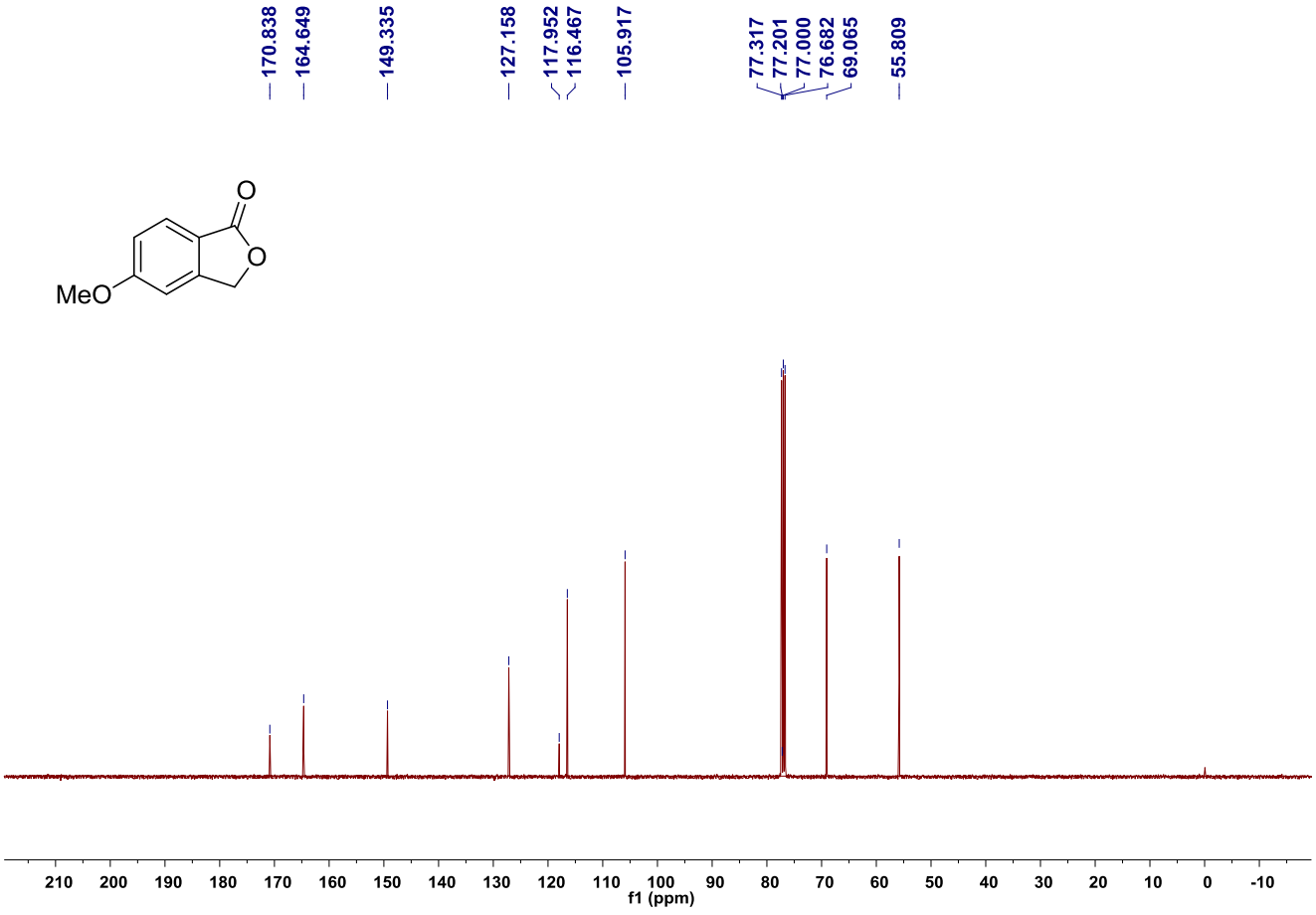
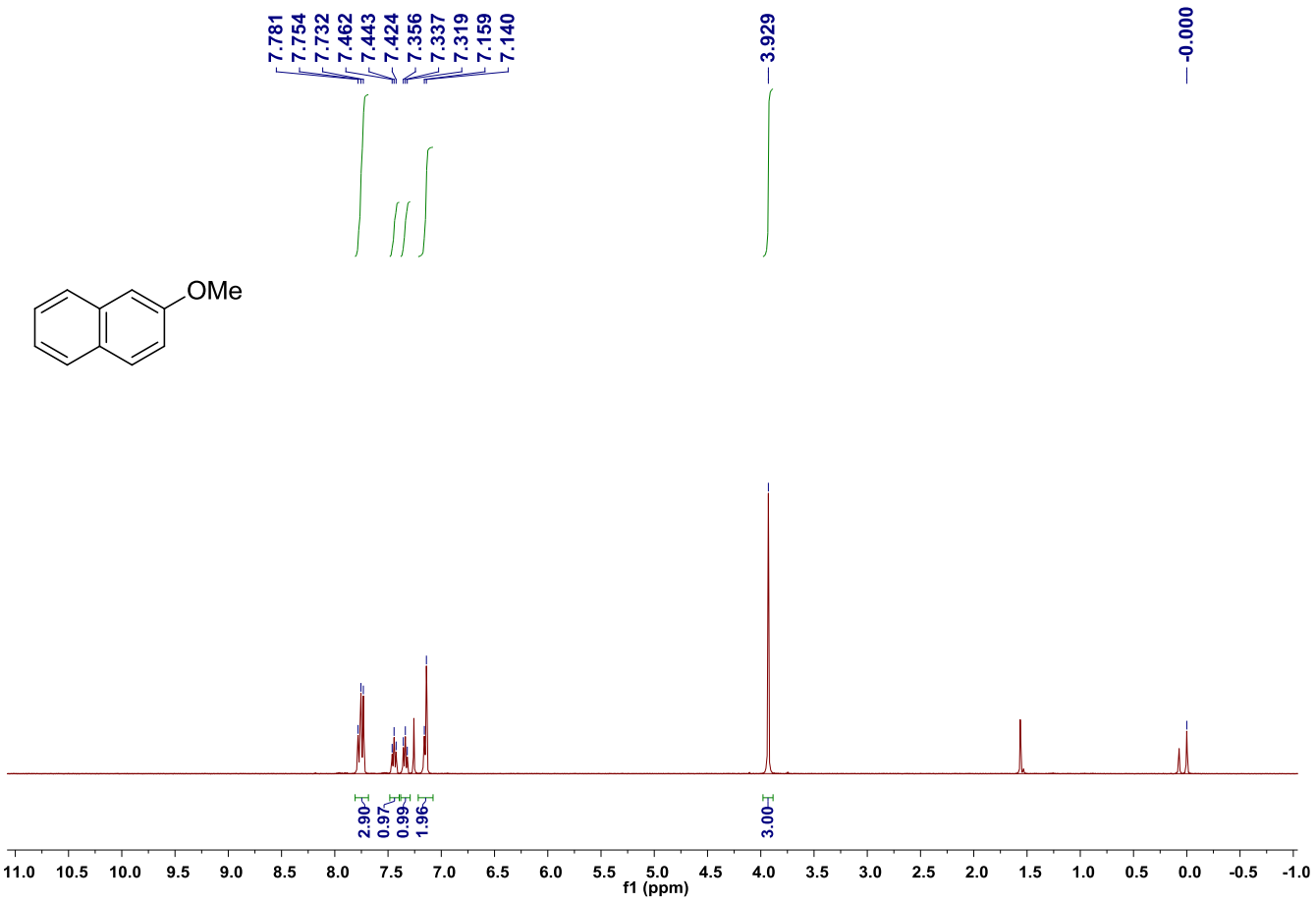
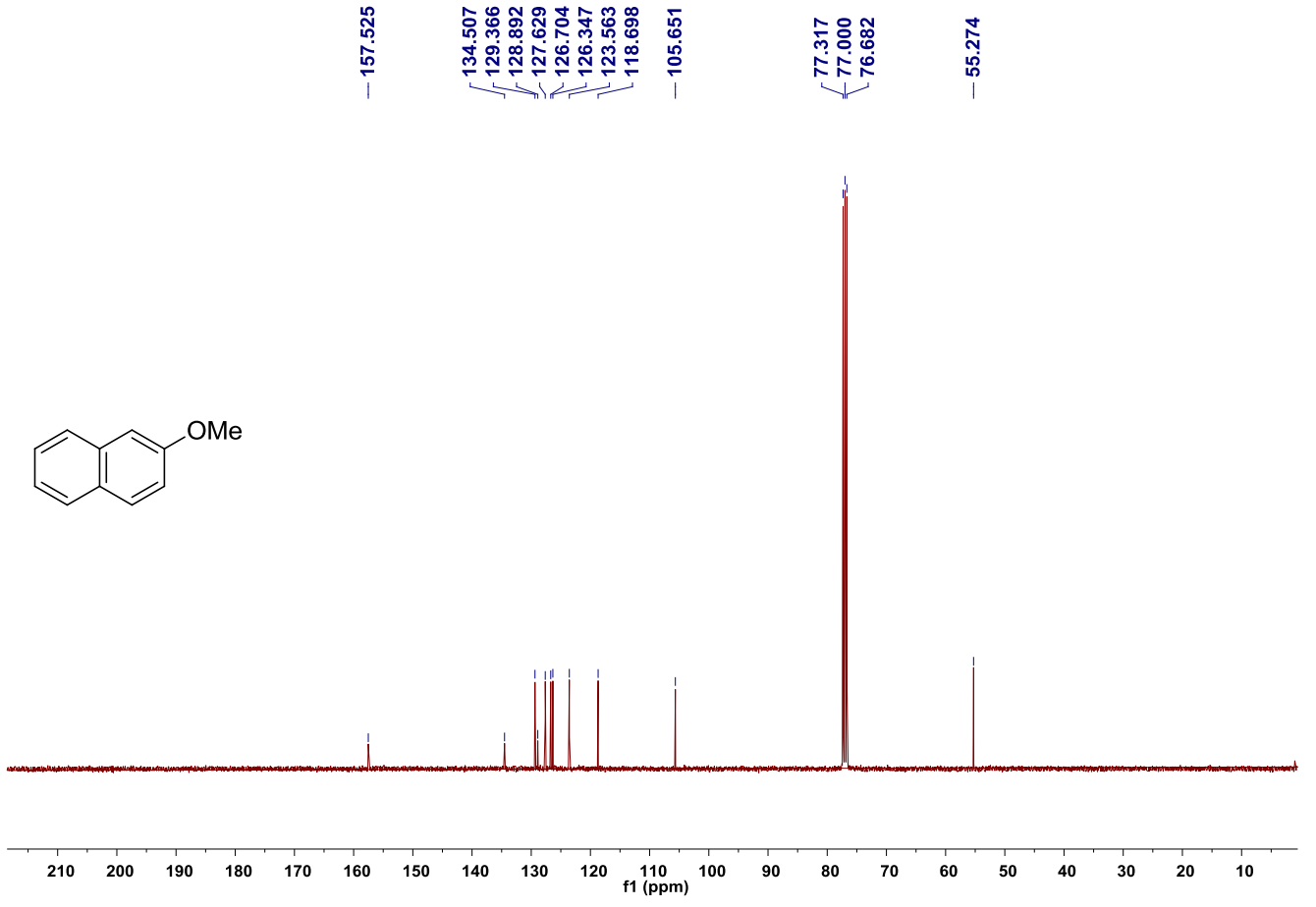
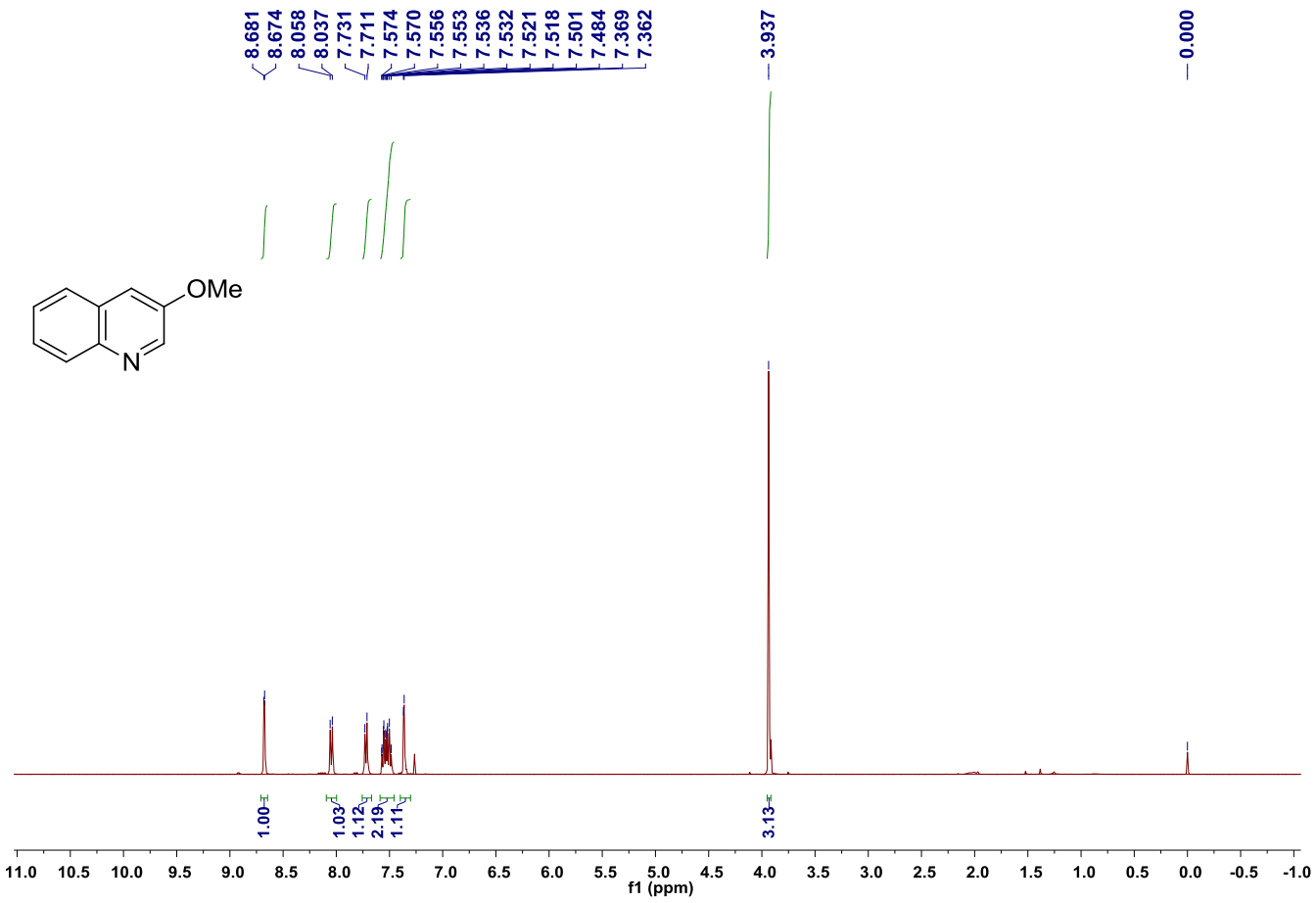
55.361
26.676
OMe
O
f1 (ppm)

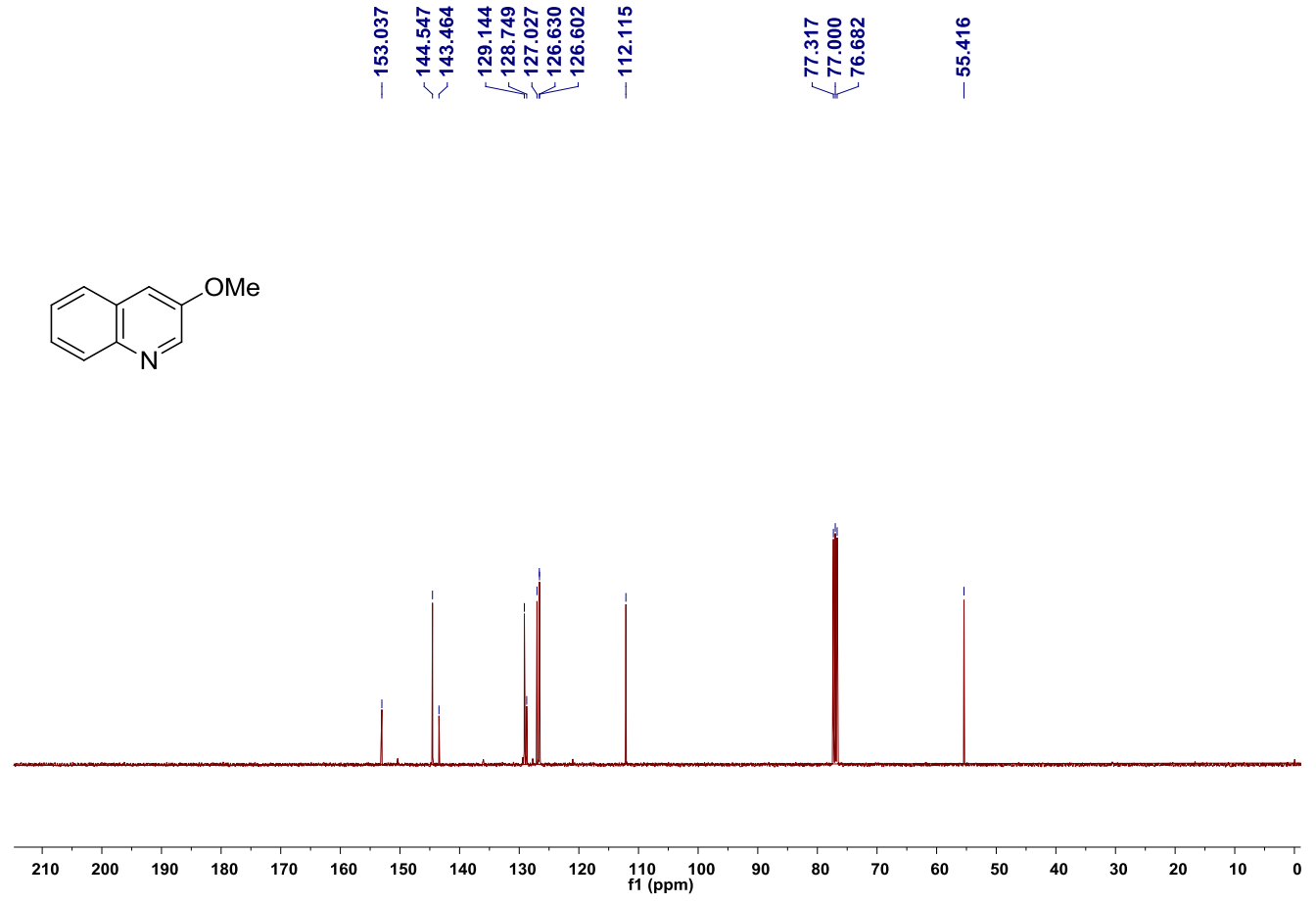

7.836
7.822
7.804
7.274
7.051
7.031
6.928
5.256
3.909
-0.000
O
O
MeO
1.00
1.01
1.00
2.00
3.05
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

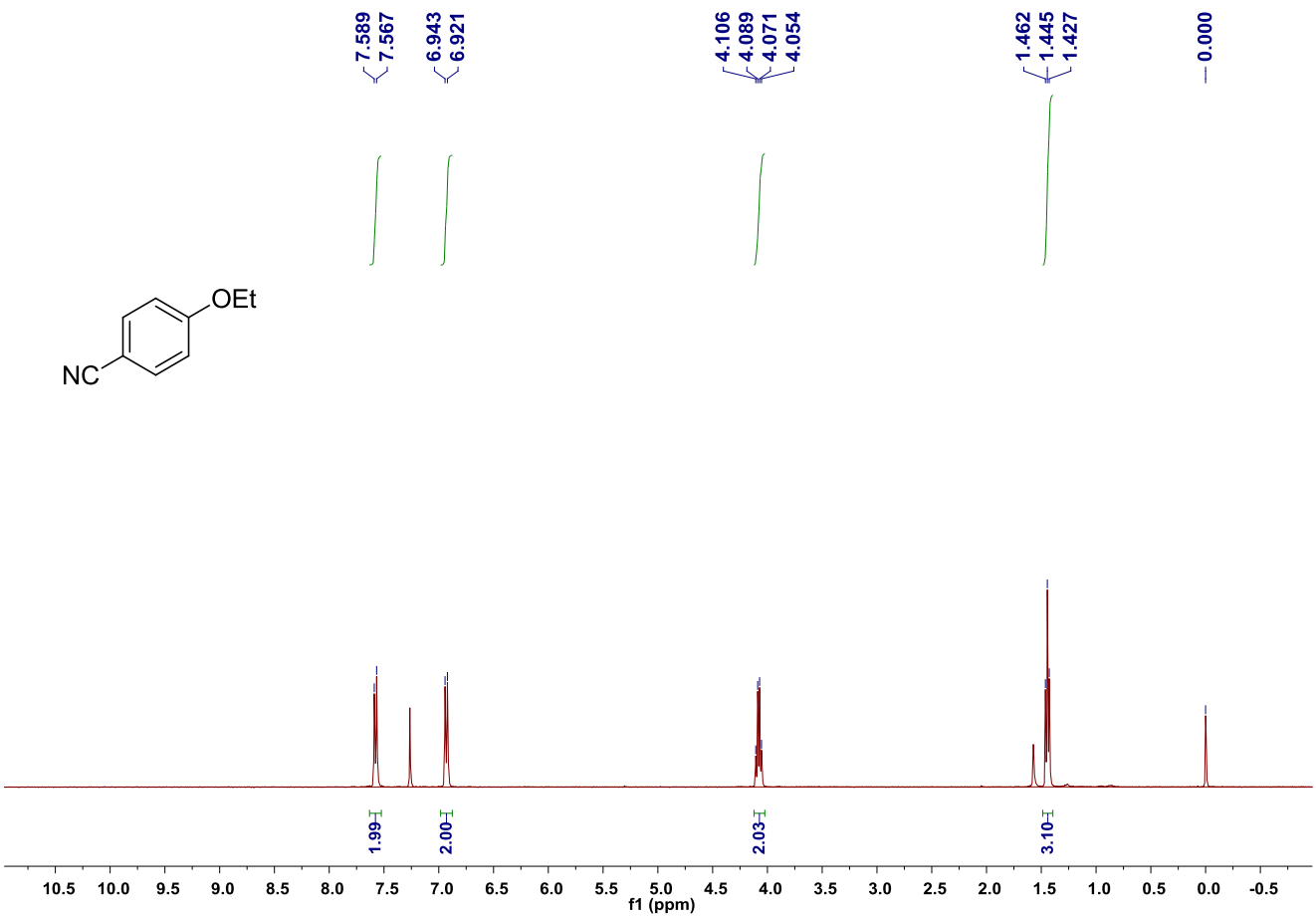

170.838
164.649
149.335
127.158
117.952
116.467
105.917
77.317
77.201
77.000
76.682
69.065
55.809
O
O
MeO
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

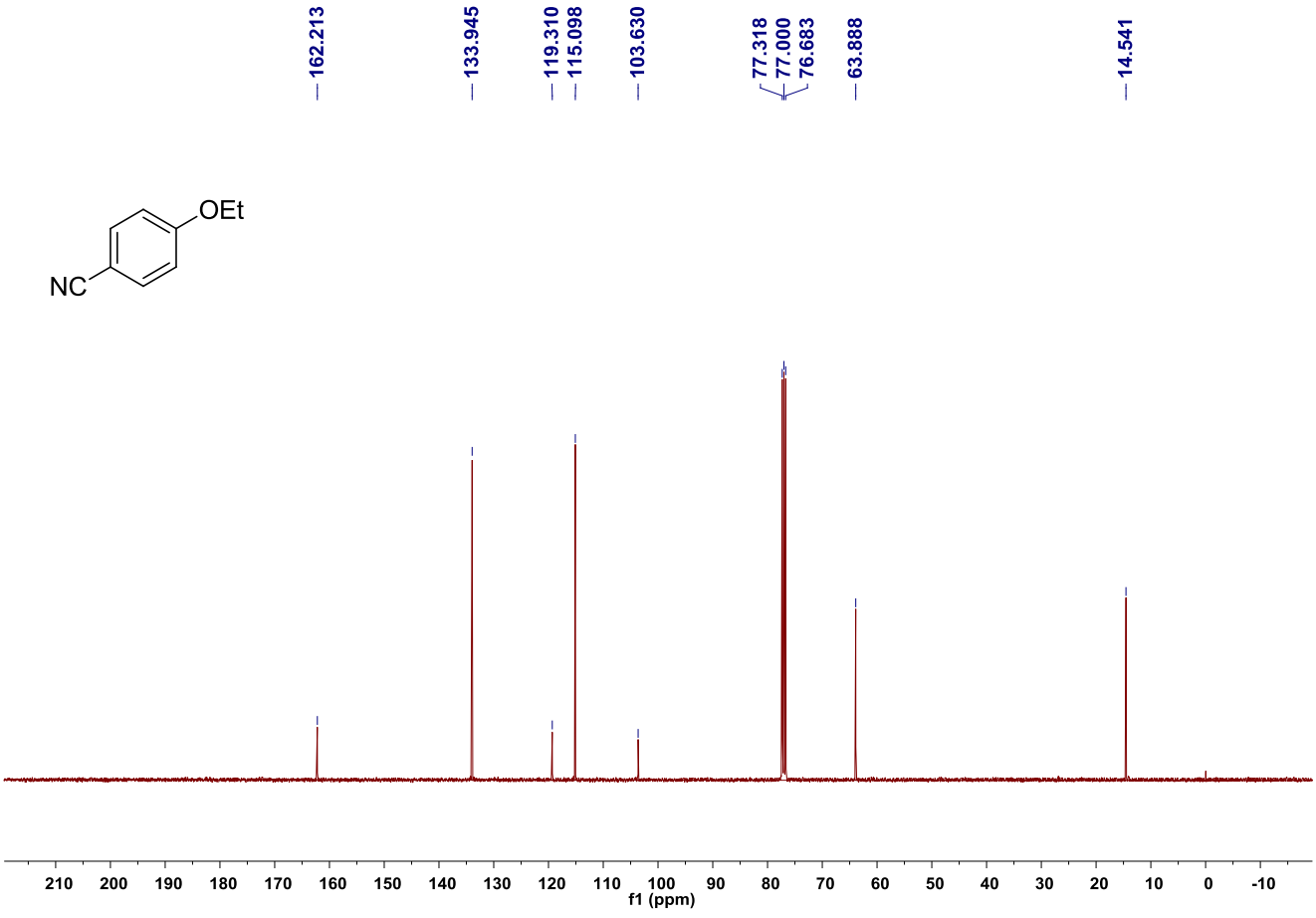

7.781
7.754
7.732
7.462
7.443
7.424
7.356
7.337
7.319
7.159
7.140
3.929
-0.000
OMe
2.90
0.97
0.99
1.96
3.00
f1 (ppm)

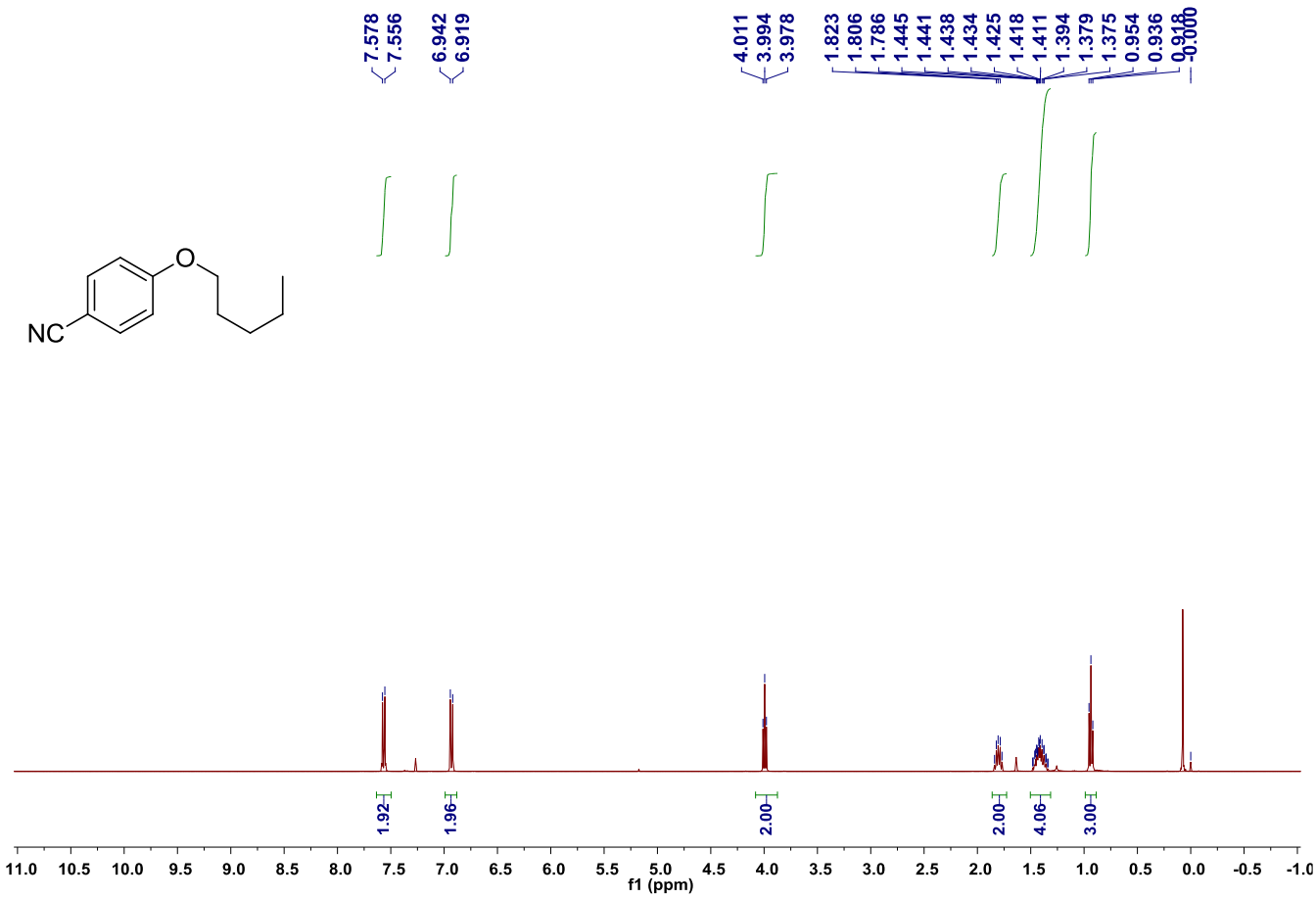

157.525
134.507
129.366
128.892
127.629
126.704
126.347
123.563
118.698
105.651
77.317
77.000
76.682
55.274
OMe
f1 (ppm)

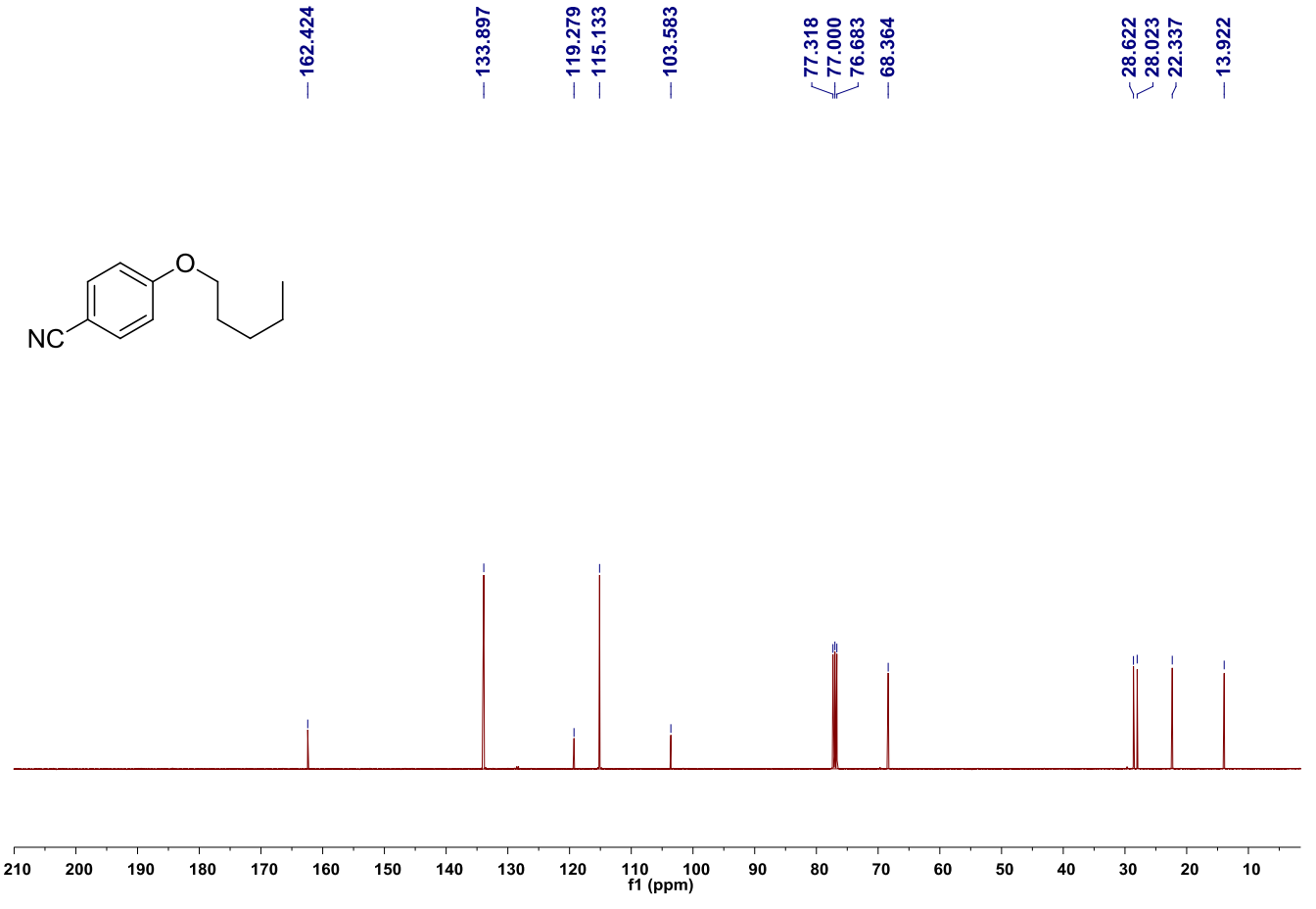

8.681
8.674
8.058
8.037
7.731
7.711
7.574
7.570
7.556
7.553
7.536
7.532
7.521
7.518
7.501
7.484
7.369
7.362
3.937
0.000
OMe
N
1.00
1.03
1.12
2.19
1.11
3.13
f1 (ppm)

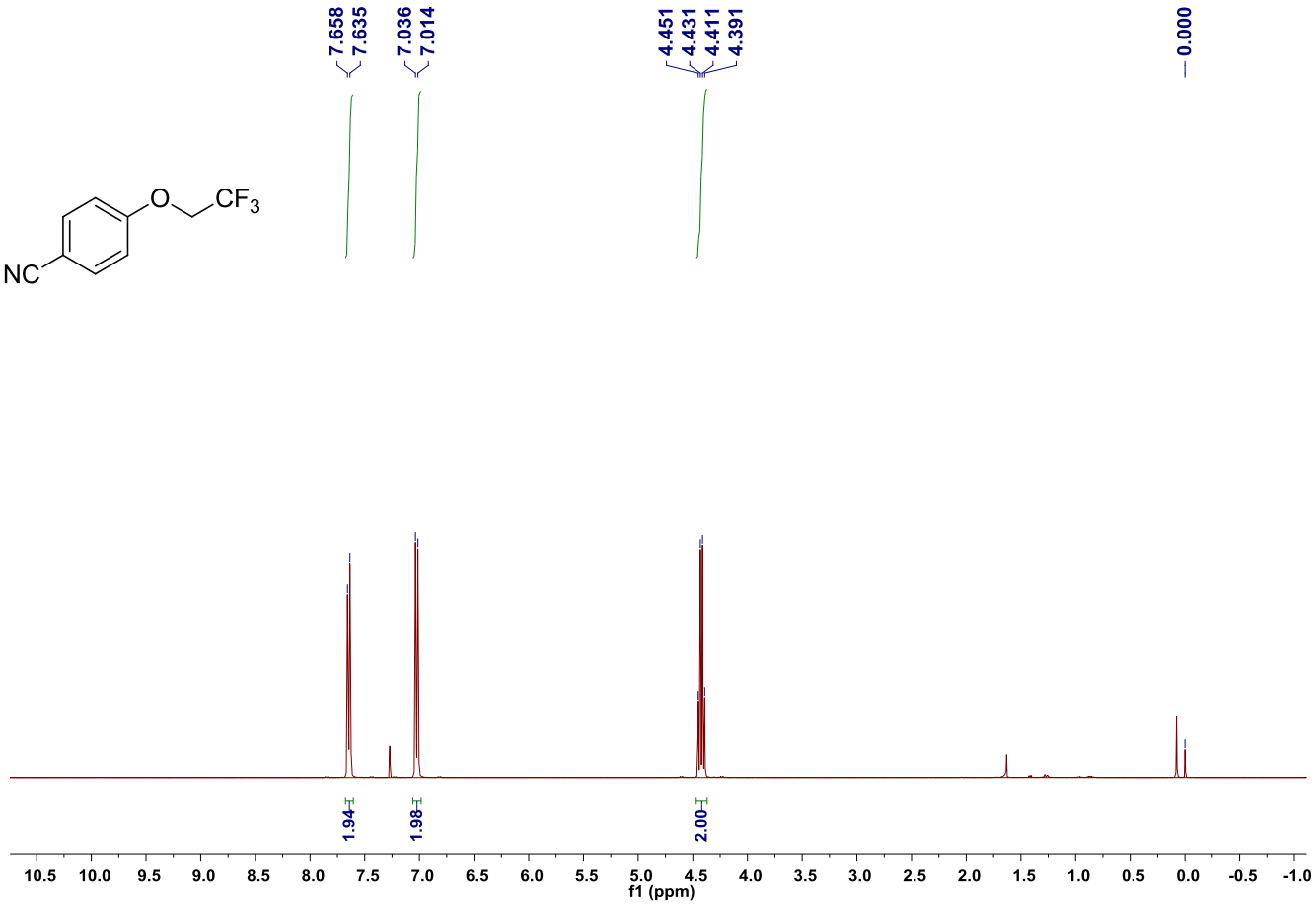

153.037
144.547
143.464
129.144
128.749
127.027
126.630
126.602
112.115
77.317
77.000
76.682
55.416
OMe
N
f1 (ppm)

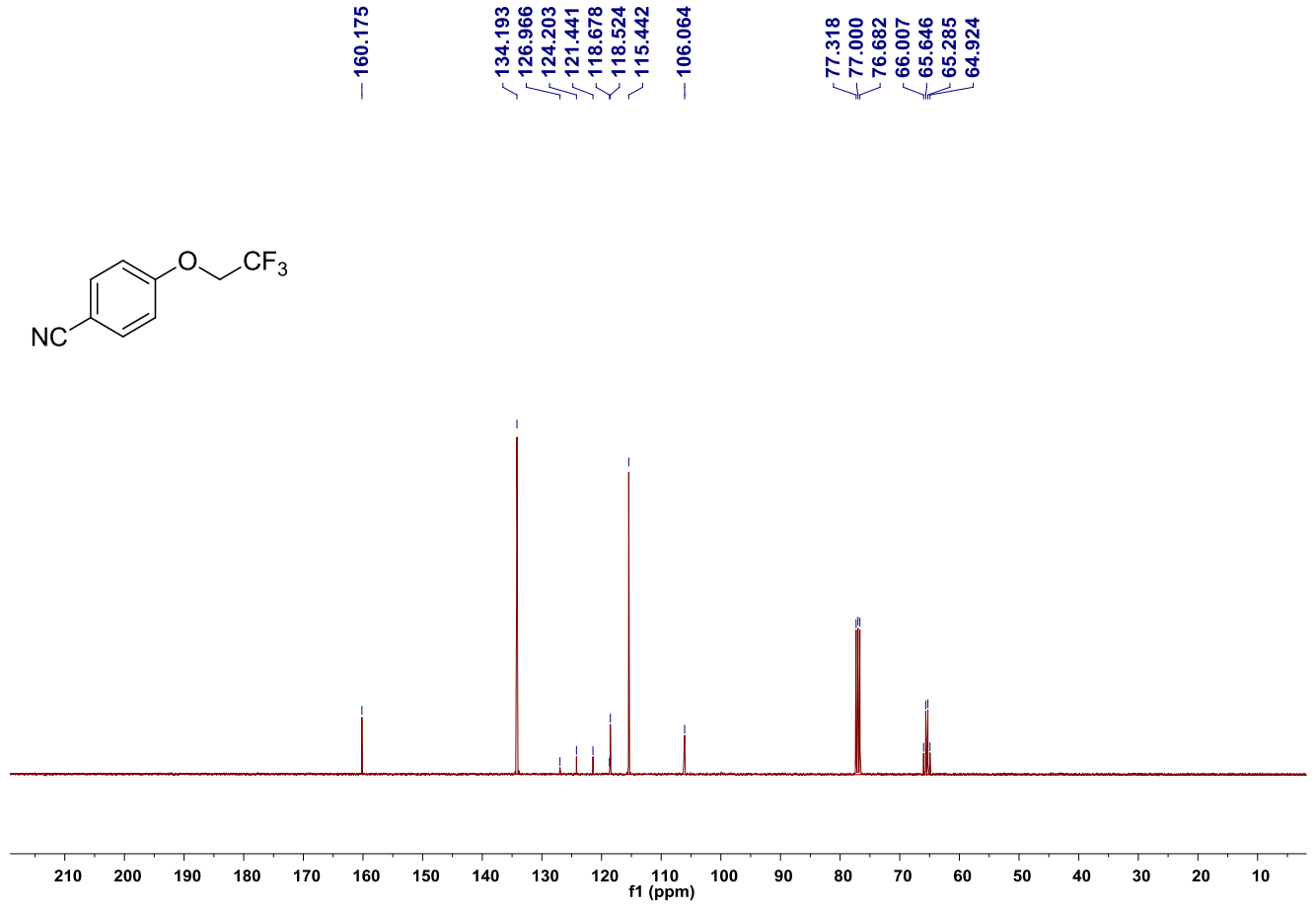

7.589
7.567
6.943
6.921
4.106
4.089
4.071
4.054
1.462
1.445
1.427
0.000
OEt
NC
1.99
2.00
2.03
3.10
f1 (ppm)

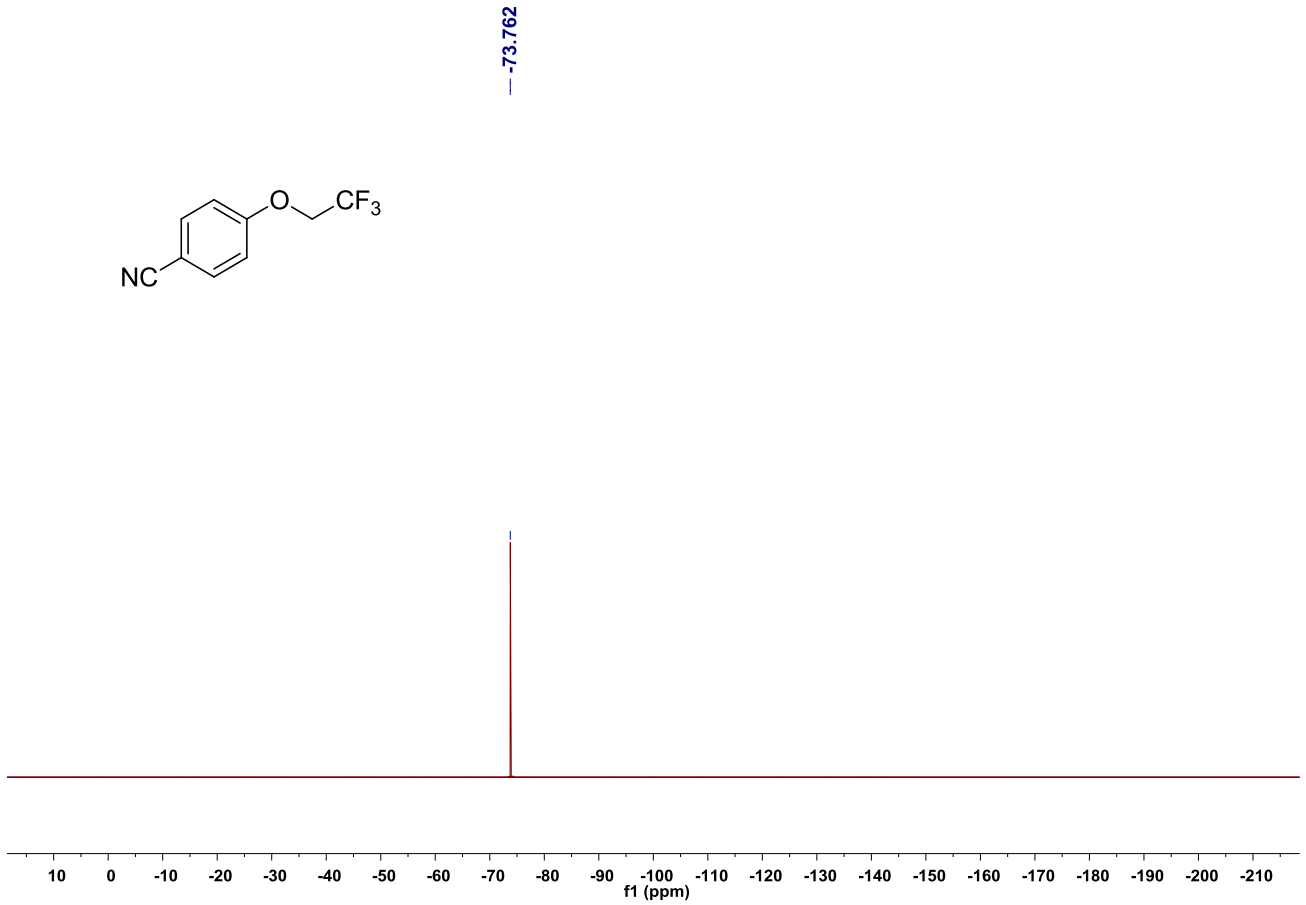

162.213
133.945
119.310
115.098
103.630
77.318
77.000
76.683
63.888
14.541
OEt
NC
f1 (ppm)

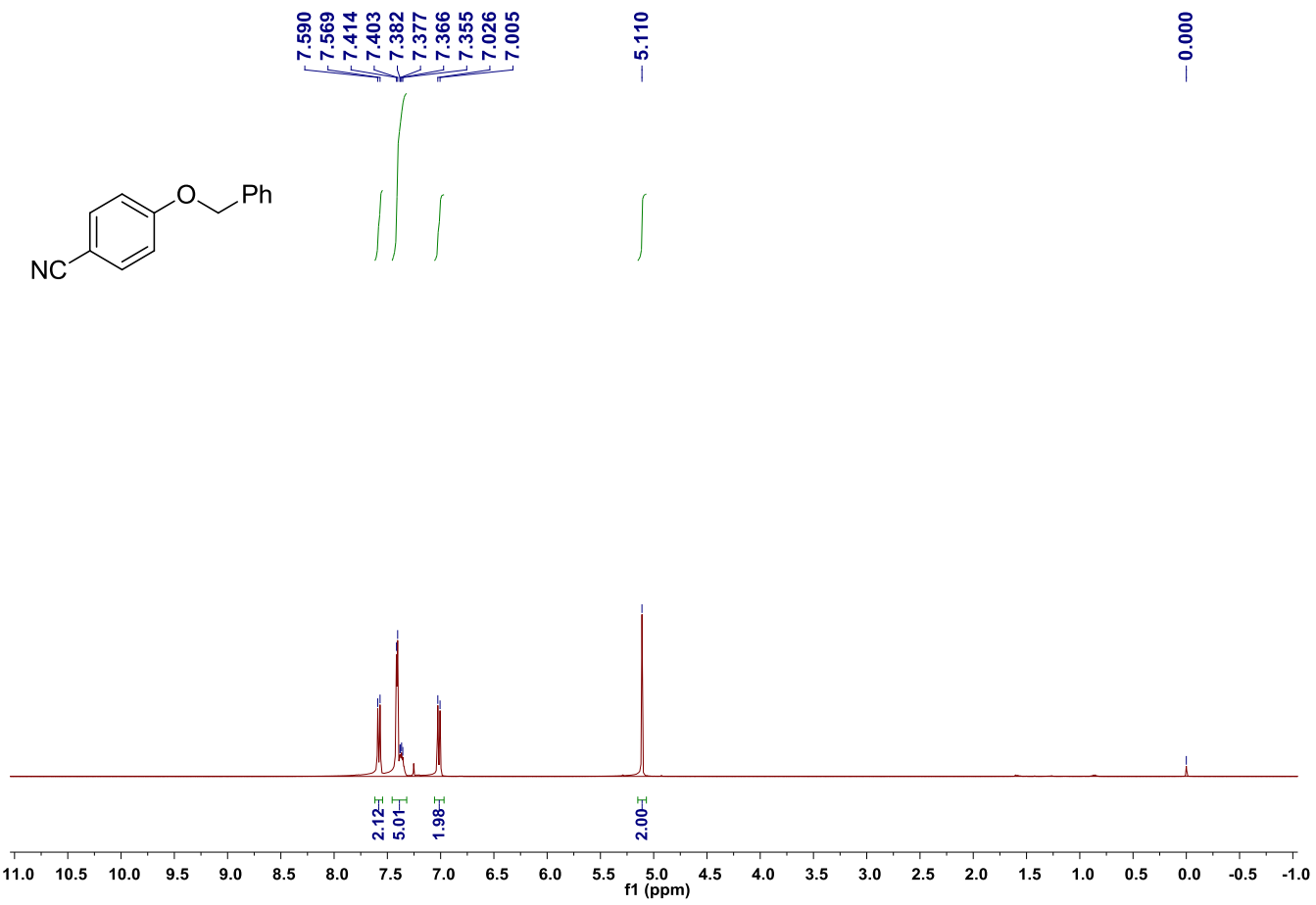

7.578
7.556
6.942
6.919
4.011
3.994
3.978
1.823
1.806
1.786
1.445
1.441
1.438
1.434
1.425
1.418
1.411
1.394
1.379
1.375
0.954
0.936
0.918
0.000
O
NC
1.92
1.96
2.00
2.00
4.06
3.00
f1 (ppm)

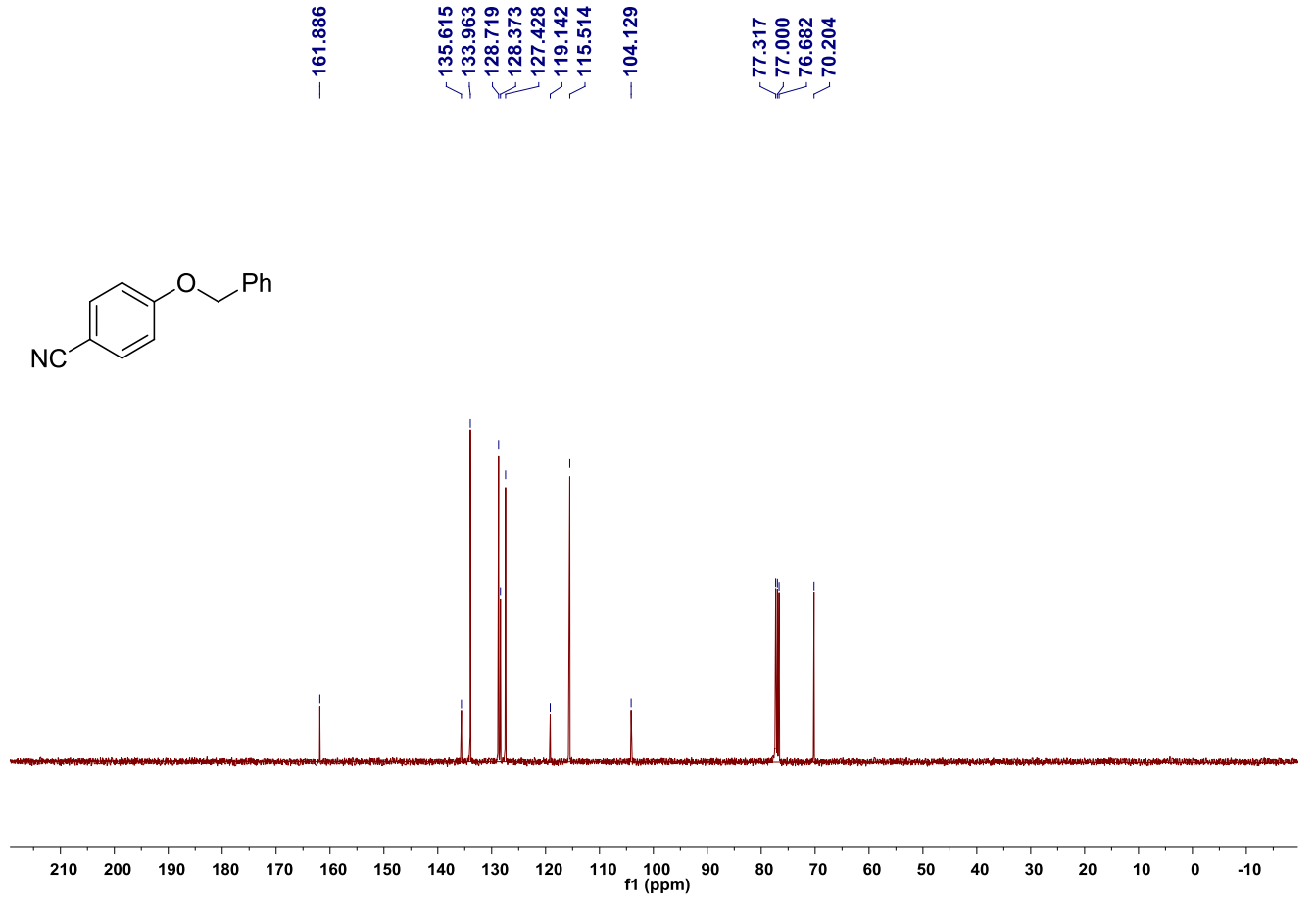

162.424
133.897
119.279
115.133
103.583
77.318
77.000
76.683
68.364
28.622
28.023
22.337
13.922
O
NC
f1 (ppm)

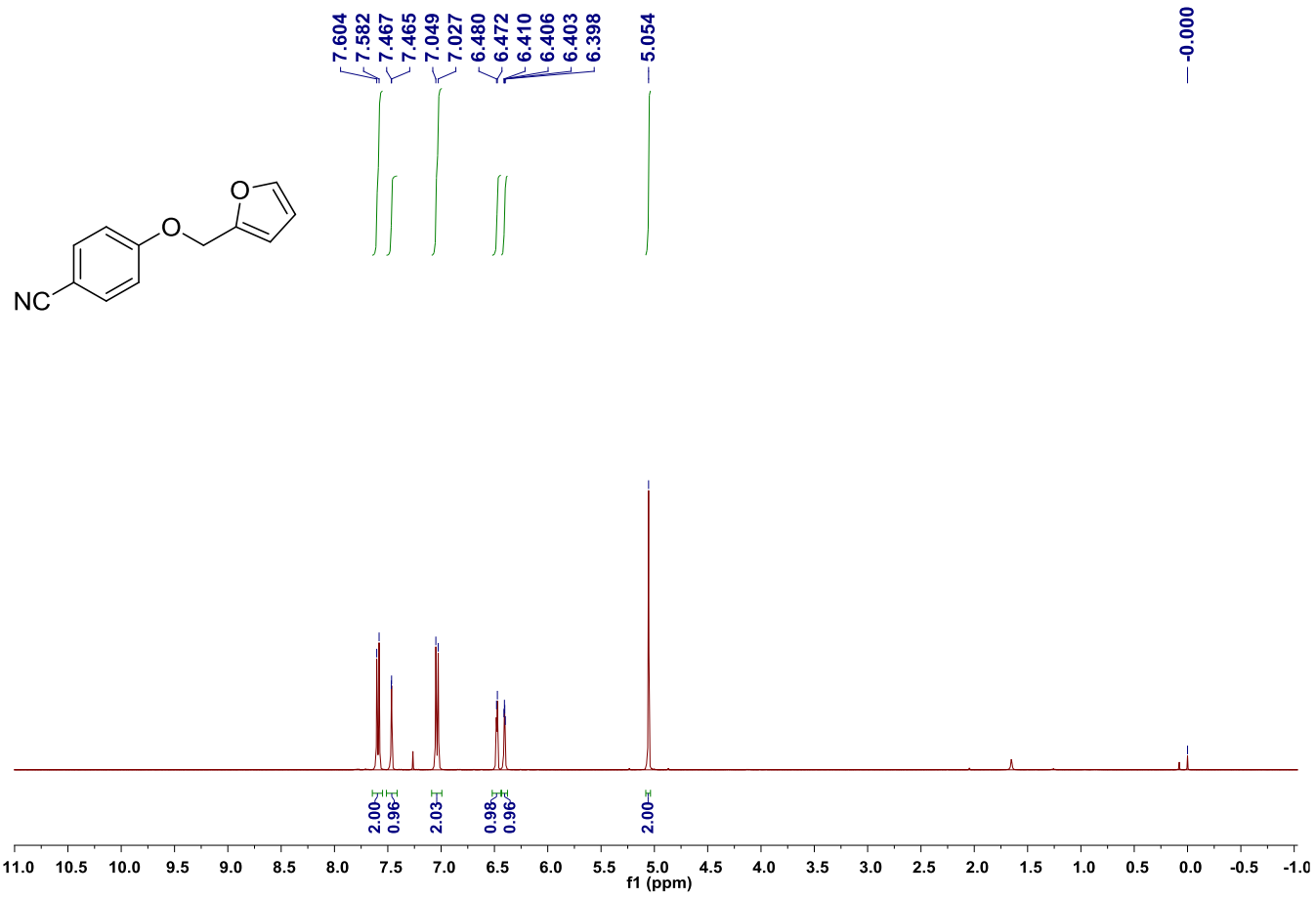

7.658
7.635
7.036
7.014
4.451
4.431
4.411
4.391
0.000
O
CF3
NC
1.94
1.98
2.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

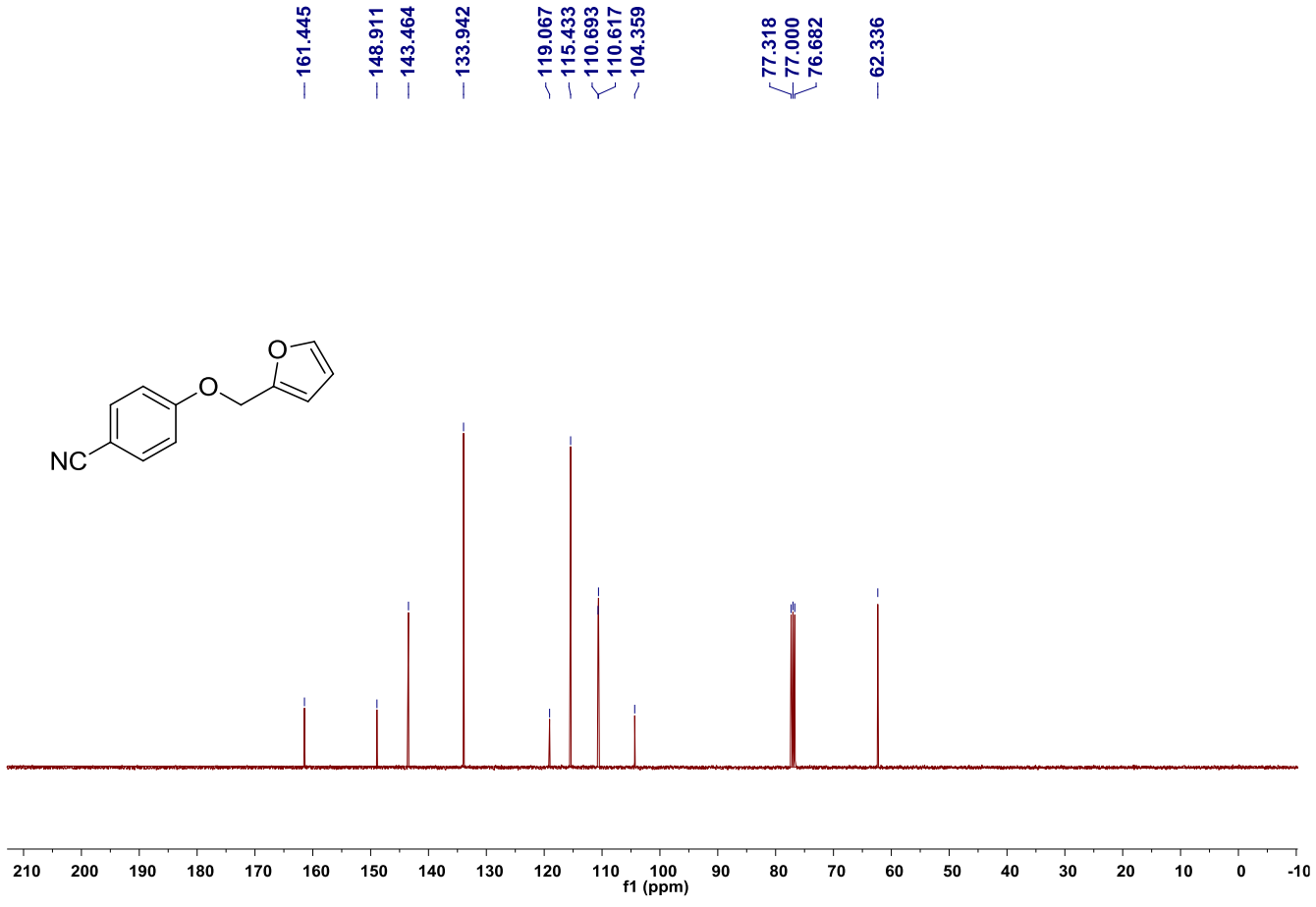

160.175
134.193
126.966
124.203
121.441
118.678
118.524
115.442
106.064
77.318
77.000
76.682
66.007
65.646
65.285
64.924
O
CF3
NC
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

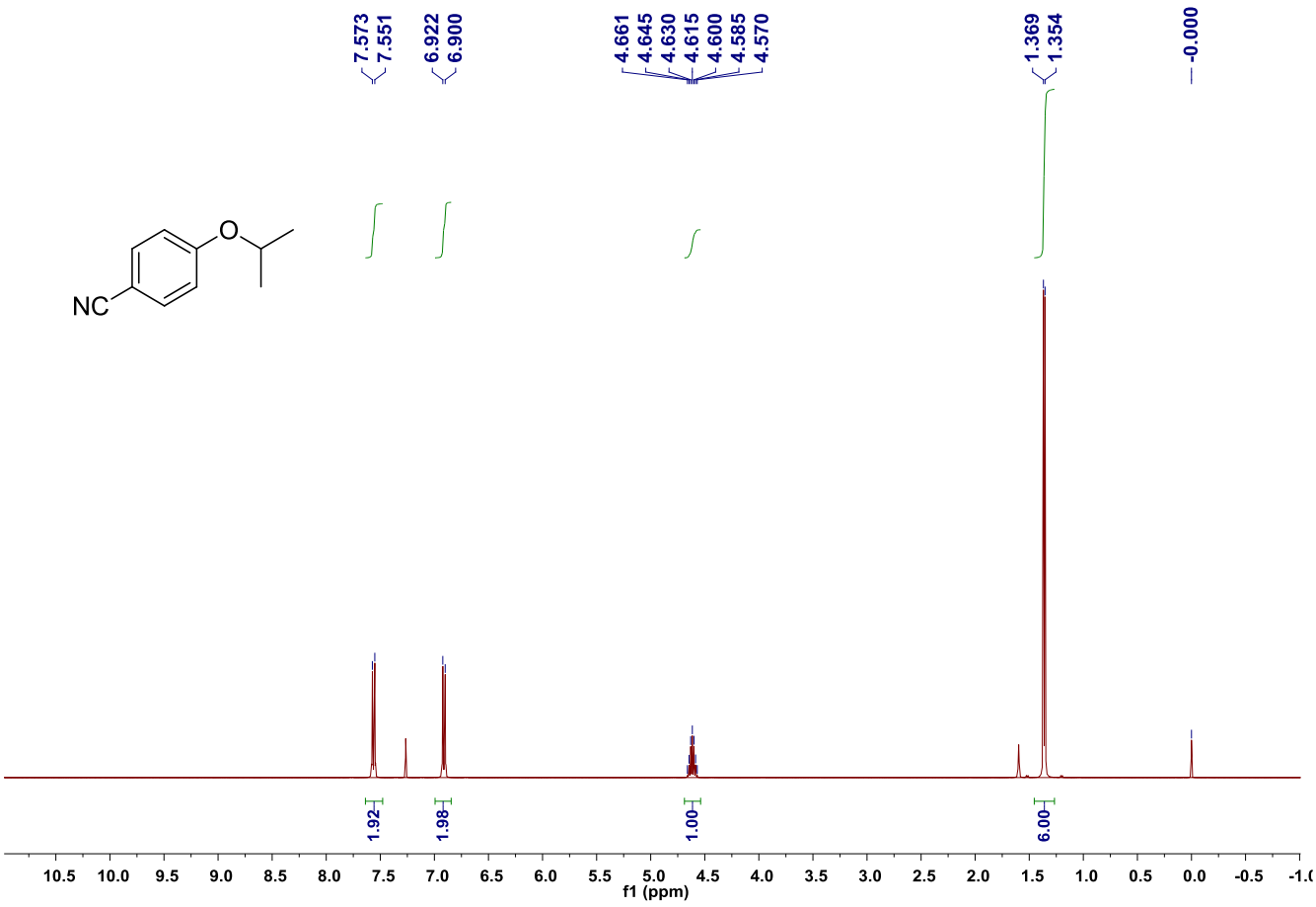

-73.762
O
CF3
NC
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

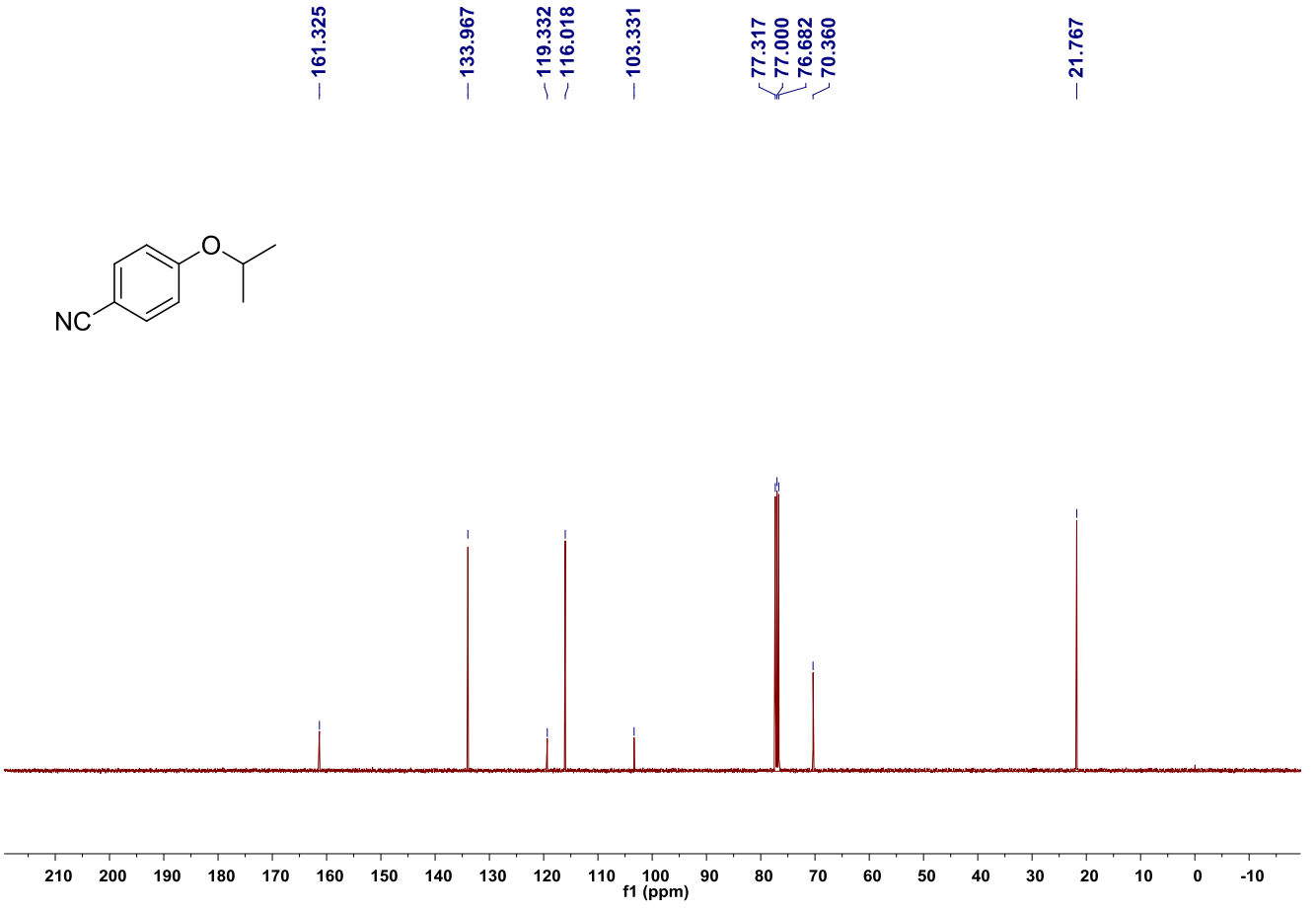

7.590
7.569
7.414
7.403
7.382
7.377
7.366
7.355
7.026
7.005
5.110
0.000
O
Ph
NC
2.12
5.01
1.98
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

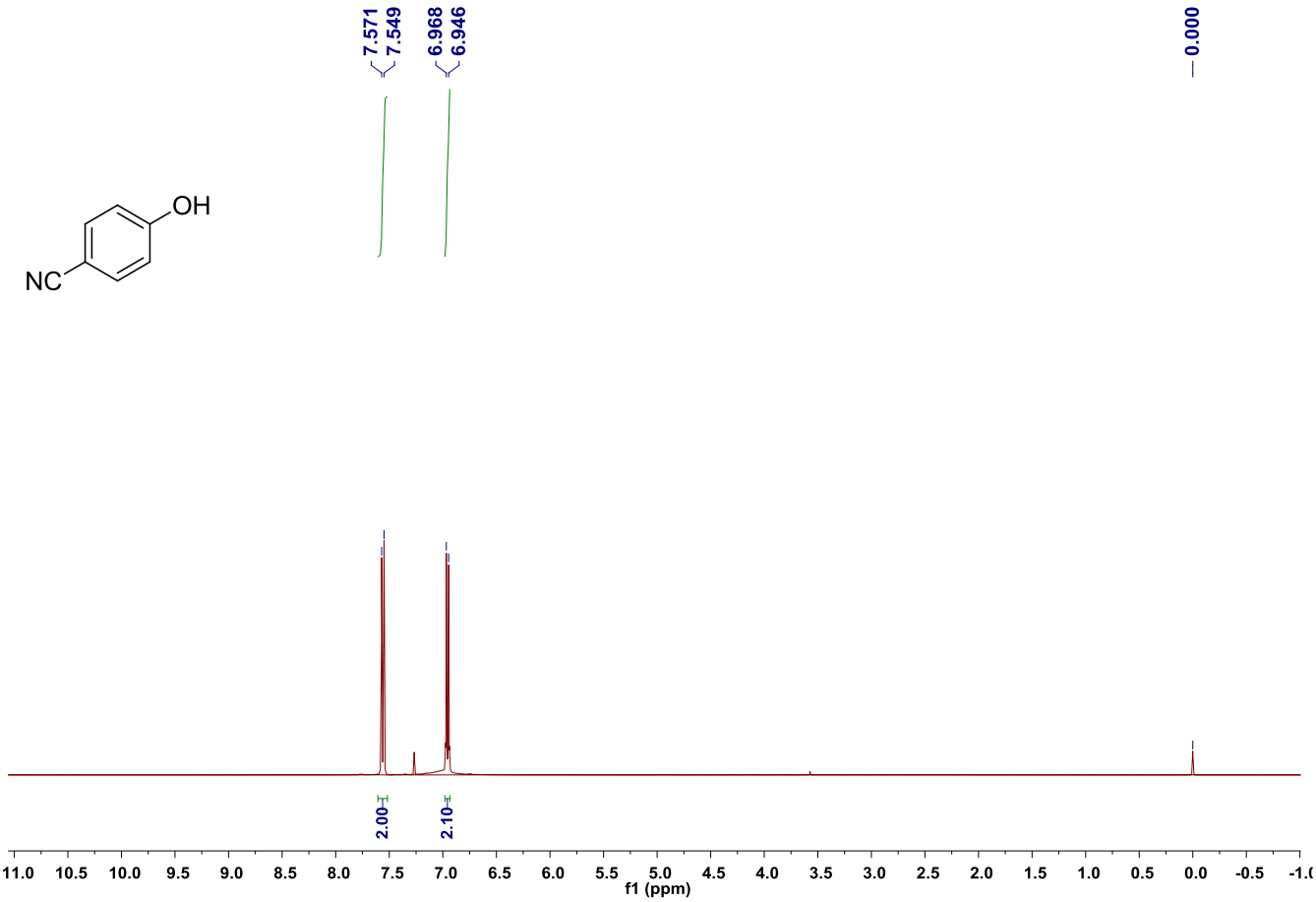

161.886
135.615
133.963
128.719
128.373
127.428
119.142
115.514
104.129
77.317
77.000
76.682
70.204
O
Ph
NC
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

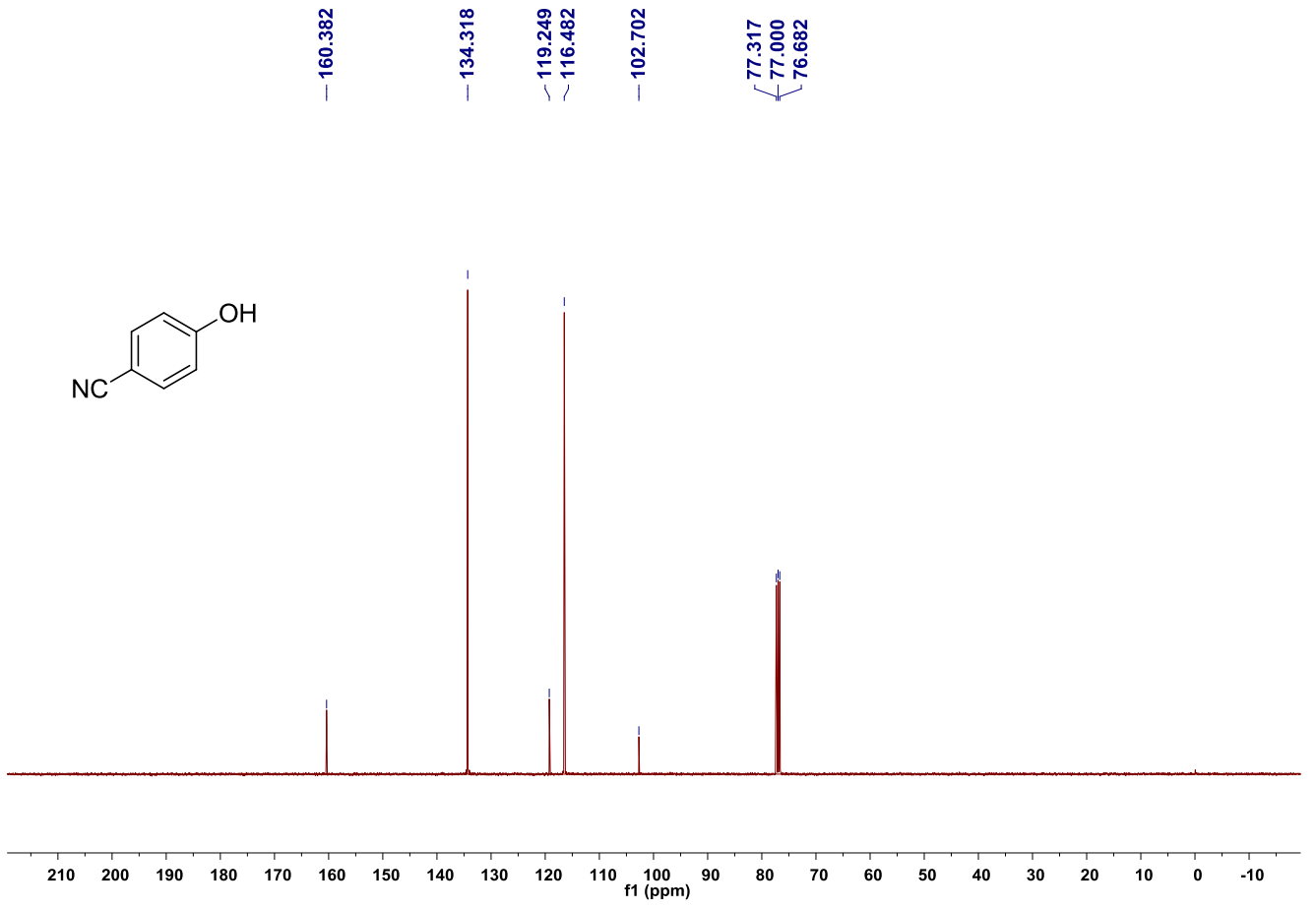

7.604
7.582
7.467
7.465
7.049
7.027
6.480
6.472
6.410
6.406
6.403
6.398
5.054
-0.000
NC
O
O
2.00
0.96
2.03
0.98
0.96
2.00
f1 (ppm)

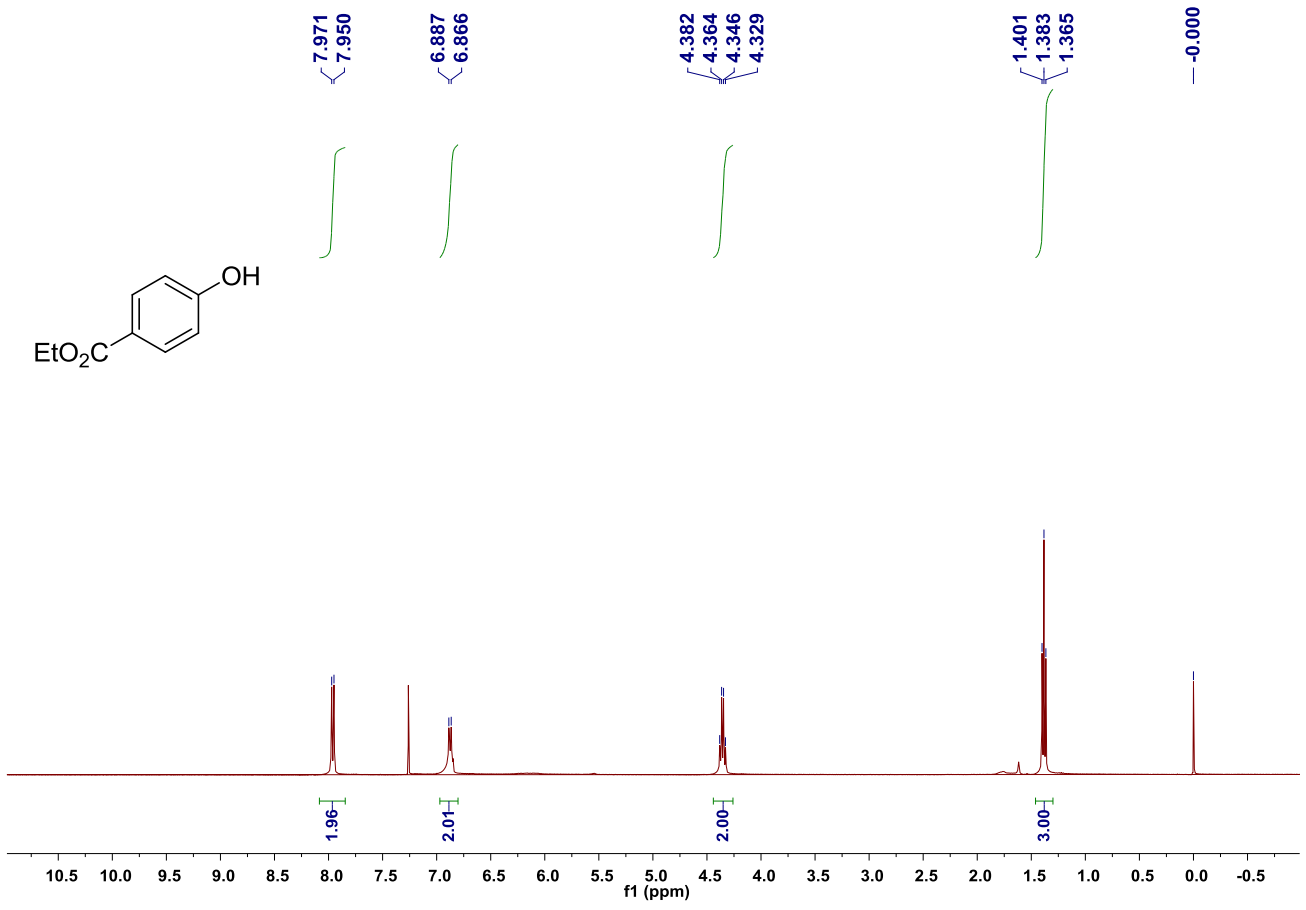

161.445
148.911
143.464
133.942
119.067
115.433
110.693
110.617
104.359
77.318
77.000
76.682
62.336
NC
O
O
f1 (ppm)

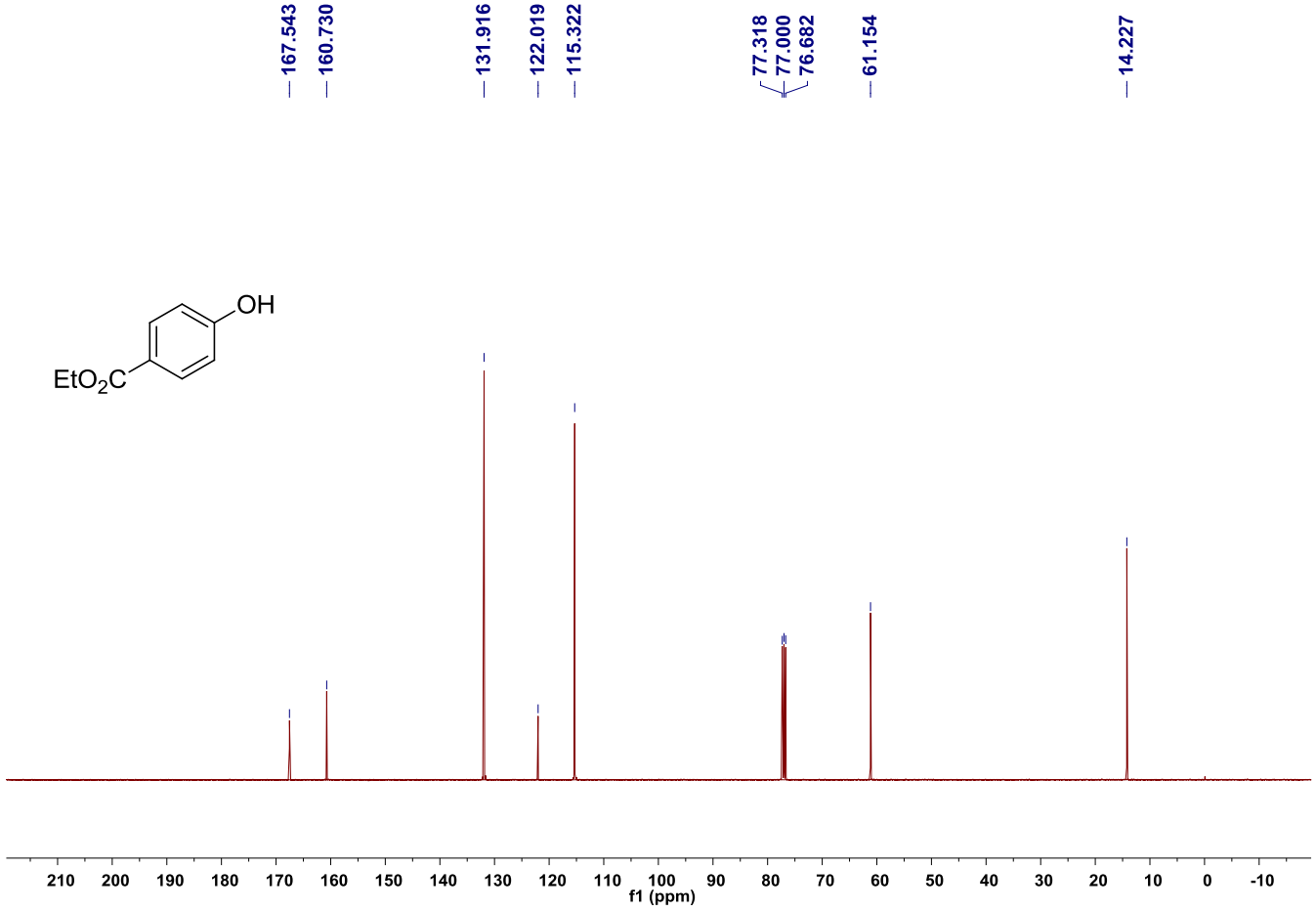

7.573
7.551
6.922
6.900
4.661
4.645
4.630
4.615
4.600
4.585
4.570
1.369
1.354
-0.000
O
NC
1.92
1.98
1.00
6.00
f1 (ppm)


161.325
133.967
119.332
116.018
103.331
77.317
77.000
76.682
70.360
21.767
O
NC
f1 (ppm)


7.571
7.549
6.968
6.946
0.000
OH
NC
2.00
2.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


160.382
134.318
119.249
116.482
102.702
77.317
77.000
76.682
OH
NC
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.971
7.950
6.887
6.866
4.382
4.364
4.346
4.329
1.401
1.383
1.365
-0.000
OH
EtO2C
1.96
2.01
2.00
3.00
f1 (ppm)


167.543
160.730
131.916
122.019
115.322
77.318
77.000
76.682
61.154
14.227
OH
EtO2C
f1 (ppm)